X
NH2
CH2
1-2

9
4
3
5
10
2
6
1
8
7
1-2

X
N
CN

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4
3
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8
11
2
6
1
10

* * * * * * * * * * Welcome to STN International * * * * * * * * * *

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	JAN 17	Pre-1988 INPI data added to MARPAT
NEWS 4	FEB 21	STN AnaVist, Version 1.1, lets you share your STN AnaVist visualization results
NEWS 5	FEB 22	The IPC thesaurus added to additional patent databases on STN
NEWS 6	FEB 22	Updates in EPFULL; IPC 8 enhancements added
NEWS 7	FEB 27	New STN AnaVist pricing effective March 1, 2006
NEWS 8	MAR 03	Updates in PATDPA; addition of IPC 8 data without attributes
NEWS 9	MAR 08	X.25 communication option no longer available after June 2006
NEWS 10	MAR 22	EMBASE is now updated on a daily basis
NEWS 11	APR 03	New IPC 8 fields and IPC thesaurus added to PATDPAFULL
NEWS 12	APR 03	Bibliographic data updates resume; new IPC 8 fields and IPC thesaurus added in PCTFULL
NEWS 13	APR 04	STN AnaVist $500 visualization usage credit offered
NEWS 14	APR 12	LINSPEC, learning database for INSPEC, reloaded and enhanced
NEWS 15	APR 12	Improved structure highlighting in FQHIT and QHIT display in MARPAT
NEWS 16	APR 12	Derwent World Patents Index to be reloaded and enhanced during second quarter; strategies may be affected
NEWS 17	MAY 10	CA/CAplus enhanced with 1900-1906 U.S. patent records
NEWS 18	MAY 11	KOREAPAT updates resume

NEWS EXPRESS	FEBRUARY 15 CURRENT VERSION FOR WINDOWS IS V8.01a, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 19 DECEMBER 2005. V8.0 AND V8.01 USERS CAN OBTAIN THE UPGRADE TO V8.01a AT http://download.cas.org/express/v8.0-Discover/
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items
NEWS IPC8	For general information regarding STN implementation of IPC 8

Enter NEWS followed by the item number or name to see news on that specific topic.

* *

COMPLETE THE STN SURVEY - APRIL 27 THROUGH MAY 31

Dear valued STN customer,

In an effort to enhance your experience with STN, we would like to better understand what you find useful. Please take approximately 5 minutes to complete a web survey.

If you provide us with your name, login ID, and e-mail address, you will be entered in a drawing to win a free iPod(R). Your responses will be kept confidential and will help us make future improvements to STN.

Take survey: http://www.zoomerang.com/survey.zgi?p=WEB2259HNKWTUW

Thank you in advance for your participation.

* * * * * * * * * * * * * * * * STN Columbus * * * * * * * * * * * * * * * *

FILE 'HOME' ENTERED AT 14:51:04 ON 15 MAY 2006

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 0.21 0.21

FILE 'REGISTRY' ENTERED AT 14:51:12 ON 15 MAY 2006
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STRUCTURE FILE UPDATES: 14 MAY 2006 HIGHEST RN 884198-07-6
DICTIONARY FILE UPDATES: 14 MAY 2006 HIGHEST RN 884198-07-6

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

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```
**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information.  *
*                                                                    *
**********************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

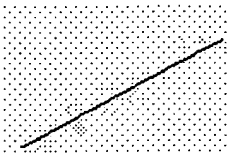
REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

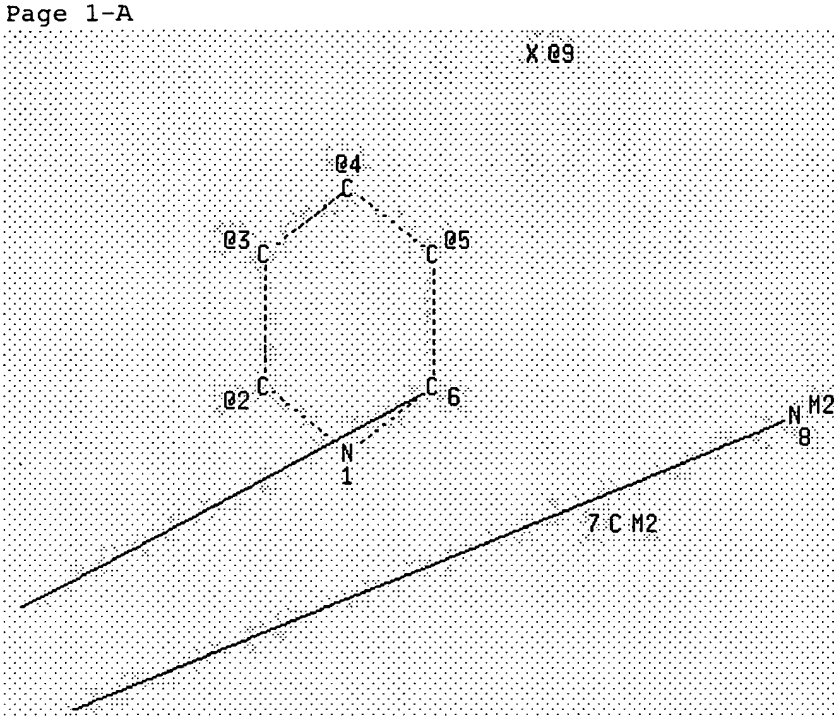
=>
Uploading structure

L1 STRUCTURE UPLOADED

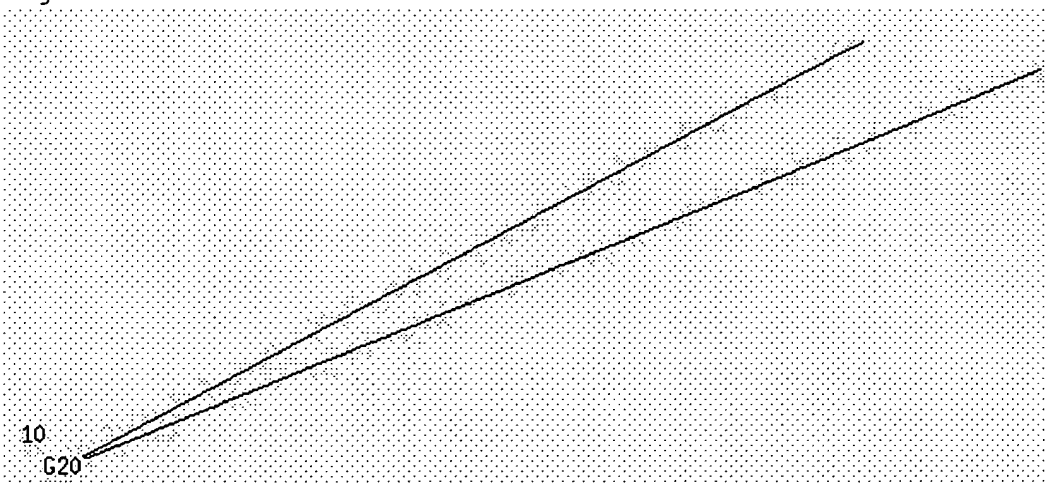
=> d l1
L1 HAS NO ANSWERS
L1 STR



Page 1-A



Page 1-B



Page 2-A

Page 2-B

```
REP G20=(1-2) 7-6 7-8
VPA 9-2/3/4/5 S
NODE ATTRIBUTES:
HCOUNT   IS M2     AT   7
HCOUNT   IS M2     AT   8
NSPEC    IS R      AT   1
NSPEC    IS R      AT   2
NSPEC    IS R      AT   3
NSPEC    IS R      AT   4
NSPEC    IS R      AT   5
```

```
NSPEC   IS R      AT   6
NSPEC   IS C      AT   7
NSPEC   IS C      AT   8
NSPEC   IS C      AT   9
NSPEC   IS C      AT  10
DEFAULT MLEVEL IS ATOM
MLEVEL  IS CLASS  AT   7  8  9
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS  10

STEREO ATTRIBUTES: NONE


=> s l1
SAMPLE SEARCH INITIATED 14:52:44 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     6687 TO ITERATE

 29.9% PROCESSED     2000 ITERATIONS                                 0 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       128838 TO   138642
PROJECTED ANSWERS:               0 TO        0

L2            0 SEA SSS SAM L1

=> s l1 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 166.50 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:52:52 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   133446 TO ITERATE

100.0% PROCESSED   133446 ITERATIONS                              64 ANSWERS
SEARCH TIME: 00.00.01

L3           64 SEA SSS FUL L1

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                 ENTRY    SESSION
FULL ESTIMATED COST                             167.82     168.03

FILE 'HCAPLUS' ENTERED AT 14:52:55 ON 15 MAY 2006
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FILE COVERS 1907 - 15 May 2006 VOL 144 ISS 21
FILE LAST UPDATED: 14 May 2006 (20060514/ED)

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

=> s l3/prep
            82 L3
       3467316 PREP/RL
L4   56 L3/PREP
                (L3 (L) PREP/RL)

=> file reg
COST IN U.S. DOLLARS   SINCE FILE   TOTAL
                                                         ENTRY   SESSION
FULL ESTIMATED COST   2.53   170.56

FILE 'REGISTRY' ENTERED AT 14:53:02 ON 15 MAY 2006
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DICTIONARY FILE UPDATES: 14 MAY 2006 HIGHEST RN 884198-07-6

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TSCA INFORMATION NOW CURRENT THROUGH January 6, 2006

  Please note that search-term pricing does apply when
  conducting SmartSELECT searches.

```
*********************************************************************
*                                                                   *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,   *
* effective March 20, 2005.  A new display format, IDERL, is now    *
* available and contains the CA role and document type information. *
*                                                                   *
*********************************************************************
```

Structure search iteration limits have been increased. See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=>

```
Uploading structure

L5      STRUCTURE UPLOADED

=>  l5
L5 IS NOT A RECOGNIZED COMMAND
The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> s l5
SAMPLE SEARCH INITIATED 14:54:03 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -     8693 TO ITERATE

 23.0% PROCESSED     2000 ITERATIONS                                19 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:       168272 TO   179448
PROJECTED ANSWERS:            1106 TO     2196

L6           19 SEA SSS SAM L5

=> s l5 full
THE ESTIMATED SEARCH COST FOR FILE 'REGISTRY' IS 166.50 U.S. DOLLARS
DO YOU WANT TO CONTINUE WITH THIS REQUEST? (Y)/N or END:y
FULL SEARCH INITIATED 14:54:08 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -   173695 TO ITERATE

100.0% PROCESSED   173695 ITERATIONS                           1726 ANSWERS
SEARCH TIME: 00.00.01

L7         1726 SEA SSS FUL L5

=> file hcaplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               167.38     337.94

FILE 'HCAPLUS' ENTERED AT 14:54:12 ON 15 MAY 2006
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FILE LAST UPDATED: 14 May 2006  (20060514/ED)
```

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=> s l7/rct
1311 L7
2847898 RCT/RL
L8 983 L7/RCT
(L7 (L) RCT/RL)

=> file hcaplus
COST IN U.S. DOLLARS SINCE FILE ENTRY 2.53 TOTAL SESSION 340.47

FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 15 MAY 2006
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FILE LAST UPDATED: 14 May 2006 (20060514/ED)

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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> s l8/rct
FIELD CODES CANNOT BE CHANGED HERE
You may have tried to apply a field code to a term that already has a field code. You can only add a field code to a term that has no field code appended to it.

=> file reg
COST IN U.S. DOLLARS SINCE FILE ENTRY 2.53 TOTAL SESSION 343.00

FILE 'REGISTRY' ENTERED AT 14:54:31 ON 15 MAY 2006
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STRUCTURE FILE UPDATES: 14 MAY 2006 HIGHEST RN 884198-07-6

```
DICTIONARY FILE UPDATES:  14 MAY 2006  HIGHEST RN 884198-07-6

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  conducting SmartSELECT searches.

**********************************************************************
*                                                                    *
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added,    *
* effective March 20, 2005.  A new display format, IDERL, is now     *
* available and contains the CA role and document type information. *
*                                                                    *
**********************************************************************

Structure search iteration limits have been increased.  See HELP SLIMITS
for details.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document.  For information
on property searching in REGISTRY, refer to:

http://www.cas.org/ONLINE/UG/regprops.html

=> d his

     (FILE 'HOME' ENTERED AT 14:51:04 ON 15 MAY 2006)

     FILE 'REGISTRY' ENTERED AT 14:51:12 ON 15 MAY 2006
L1             STRUCTURE UPLOADED
L2           0 S L1
L3          64 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:52:55 ON 15 MAY 2006
L4          56 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:53:02 ON 15 MAY 2006
L5             STRUCTURE UPLOADED
L6          19 S L5
L7        1726 S L5 FULL

     FILE 'HCAPLUS' ENTERED AT 14:54:12 ON 15 MAY 2006
L8         983 S L7/RCT

     FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 15 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:54:31 ON 15 MAY 2006

=> file hcaplus
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
                                               ENTRY    SESSION
FULL ESTIMATED COST                             0.44     343.44

FILE 'HCAPLUS' ENTERED AT 14:54:37 ON 15 MAY 2006
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
```

FILE COVERS 1907 - 15 May 2006 VOL 144 ISS 21
FILE LAST UPDATED: 14 May 2006 (20060514/ED)

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This file contains CAS Registry Numbers for easy and accurate
substance identification.

```
=> d his

     (FILE 'HOME' ENTERED AT 14:51:04 ON 15 MAY 2006)

     FILE 'REGISTRY' ENTERED AT 14:51:12 ON 15 MAY 2006
L1             STRUCTURE UPLOADED
L2           0 S L1
L3          64 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:52:55 ON 15 MAY 2006
L4          56 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:53:02 ON 15 MAY 2006
L5             STRUCTURE UPLOADED
L6          19 S L5
L7        1726 S L5 FULL

     FILE 'HCAPLUS' ENTERED AT 14:54:12 ON 15 MAY 2006
L8         983 S L7/RCT

     FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 15 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:54:31 ON 15 MAY 2006

     FILE 'HCAPLUS' ENTERED AT 14:54:37 ON 15 MAY 2006

=> s l8 and l4
L9          30 L8 AND L4

=> s l9 and vangelisti, m?/au
            3 VANGELISTI, M?/AU
L10         1 L9 AND VANGELISTI, M?/AU

=> d l10, ibib abs hitstr, 1

L10  ANSWER 1 OF 1  HCAPLUS  COPYRIGHT 2006 ACS on STN
```

Full Text | Other References

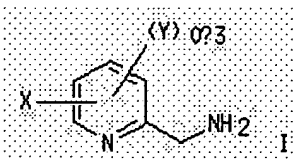
```
ACCESSION NUMBER:        2004:427623  HCAPLUS
```

DOCUMENT NUMBER: 141:7024
TITLE: A novel process for the preparation of 2-aminomethylpyridine derivatives via Ni-catalized hydrogenation of 2-cyanopyridine derivatives
INVENTOR(S): **Vangelisti, Manuel**
PATENT ASSIGNEE(S): Bayer Cropscience Sa, Fr.
SOURCE: Eur. Pat. Appl., 6 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1422221	A1	20040526	EP 2002-356236	20021120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
WO 2004046114	A1	20040603	WO 2003-EP14892	20031118
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003290121	A1	20040615	AU 2003-290121	20031118
BR 2003014461	A	20050726	BR 2003-14461	20031118
EP 1565440	A1	20050824	EP 2003-782483	20031118
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006508143	T2	20060309	JP 2004-552709	20031118
US 2006004206	A1	20060105	US 2005-535723	20050520

PRIORITY APPLN. INFO.:			EP 2002-356236	A 20021120
			WO 2003-EP14892	W 20031118

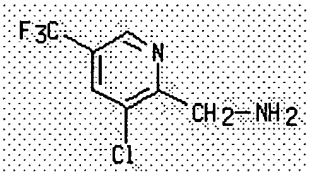
OTHER SOURCE(S): CASREACT 141:7024; MARPAT 141:7024
GI



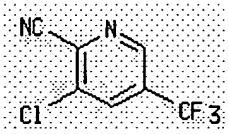
AB The invention relates to a process for the prepn. of 2-aminomethylpyridine derivs. of formula I [wherein: X is halogen atom; each Y may be the same or different and may be a halogen atom, a halogenoalkyl, an alkoxycarbonyl or an alkylsulfonyl], useful as intermediates for prepn. of pesticides. 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine was prepd. via Raney Ni-catalized hydrogenation of 2-cyano-3-chloro-5-trifluoromethylpyridine with a yield of 97%. The advantages of the proposed prepn. of 2-aminomethylpyridine derivs. include the use of Raney nickel catalyst instead of expensive Pd catalyst (the Pd-catalized hydrogenation suffers from the disadvantage of dehalogenation reaction; Pd is also very sensitive to catalysts poisons).

IT **175277-74-4P**

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(novel process for the prepn. of aminomethylpyridine derivs. via Raney Ni-catalized hydrogenation of cyanopyridine derivs.)
RN 175277-74-4 HCAPLUS
CN 2-Pyridinemethanamine, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT **80194-70-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(reactant; novel process for the prepn. of aminomethylpyridine derivs. via Raney Ni-catalized hydrogenation of cyanopyridine derivs.)
RN 80194-70-3 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d his

(FILE 'HOME' ENTERED AT 14:51:04 ON 15 MAY 2006)

FILE 'REGISTRY' ENTERED AT 14:51:12 ON 15 MAY 2006
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 64 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:52:55 ON 15 MAY 2006
L4 56 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:53:02 ON 15 MAY 2006
L5 STRUCTURE UPLOADED
L6 19 S L5
L7 1726 S L5 FULL

FILE 'HCAPLUS' ENTERED AT 14:54:12 ON 15 MAY 2006
L8 983 S L7/RCT

FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 15 MAY 2006

FILE 'REGISTRY' ENTERED AT 14:54:31 ON 15 MAY 2006

FILE 'HCAPLUS' ENTERED AT 14:54:37 ON 15 MAY 2006
L9 30 S L8 AND L4
L10 1 S L9 AND VANGELISTI, M?/AU

```
=> s l9 not l10
L11         29 L9 NOT L10

=> d l11, ibib abs hitstr, 1-29

L11  ANSWER 1 OF 29  HCAPLUS  COPYRIGHT 2006 ACS on STN
```

Full Text | Cited References

```
ACCESSION NUMBER:         2006:104503  HCAPLUS
DOCUMENT NUMBER:          144:192119
TITLE:                    Preparation of substituted arylamine derivatives,
                          particularly 2-aminonicotinamides, as antitumor agents
INVENTOR(S):              Yuan, Chester Chenguang; Yang, Kevin; Vanderplas,
                          Simon; Riahi, Babak; Potashman, Michele; Patel, Vinod
                          F.; Nomak, Rana; Li, Aiwen; Huang, Qi; Harmange,
                          Jean-Christophe; Askew, Benny C., Jr.
PATENT ASSIGNEE(S):       Amgen Inc., USA
SOURCE:                   PCT Int. Appl., 351 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.           KIND   DATE        APPLICATION NO.          DATE
     ---------------      ----   --------    --------------------     --------
     WO 2006012374         A1    20060202    WO 2005-US25800          20050720
         W:  AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ,
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             KG, KZ, MD, RU, TJ, TM
     US 2006040966         A1    20060223    US 2005-185556           20050719
PRIORITY APPLN. INFO.:                       US 2004-590544P      P   20040722
                                             US 2005-185556       A2  20050719

OTHER SOURCE(S):          MARPAT 144:192119
GI
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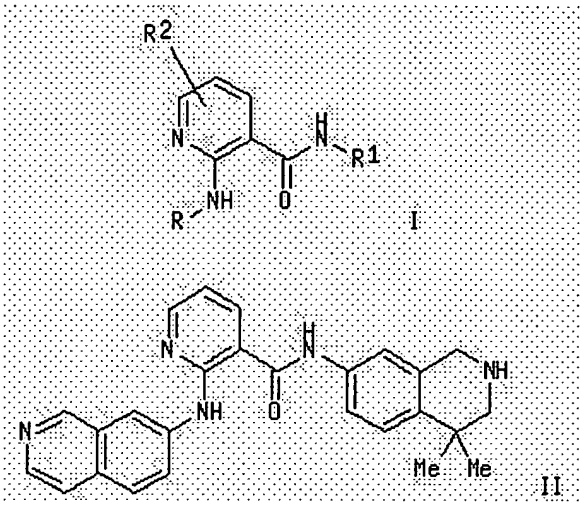

AB Title compds. I [R = (un)substituted 9- or 10-membered heterocyclyl selected from 7-isoquinolinyl, 1-oxo-2,3-dihydrobenzofuran-4-yl, 1,6-naphthyridin-3-yl, etc.; R1 = (un)substituted Ph, 5-6 membered heteroaryl, 9-10 membered bicyclic heterocyclyl, 11-14 membered tricyclic heterocyclyl; R2 = H, halo, halo/alkyl], and their analogs, and their pharmaceutically acceptable derivs., are prepd. and disclosed as agents effective for treatment of angiogenesis and related diseases such as cancer. Thus, acylation of 7-amino-4,4-dimethyl-3,4-dihydro-1H-isoquinoline-2-carboxylic acid tert-Bu ester with 2-chloropyridine-3-carbonyl chloride, followed by amination of the chloride intermediate (no data) with 7-aminoisoquinoline and deprotection gave amide II?HCl. Selected I inhibited VEGF-stimulated HUVEC proliferation at a level below 1 μM. In the tumor model, I are active at doses less than 150 mpk.

IT **97509-75-6P 312904-51-1P 561297-96-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of substituted aminonicotinamides as antitumor agents)

RN 97509-75-6 HCAPLUS
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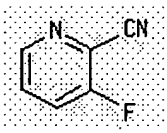

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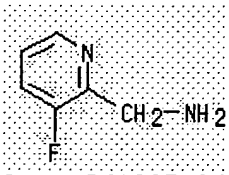

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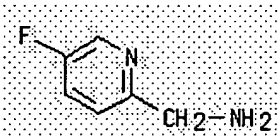

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 2 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:1331127 HCAPLUS
DOCUMENT NUMBER: 144:69727
TITLE: Preparation of tartaric acid functional compounds for the treatment of inflammatory disorders
INVENTOR(S): Guo, Zhuyan; Orth, Peter; Zhu, Zhaoning; Mazzola, Robert D.; Chan, Tin Yau; Vaccaro, Henry A.; McKittrick, Brian; Kozlowski, Joseph A.; Lavey, Brian J.; Zhou, Guowei; Paliwal, Sunil; Wong, Shing-Chun; Shih, Neng-Yang; Ting, Pauline C.; Rosner, Kristin E.; Shipps, Gerald W. Jr.; Siddiqui, M. Arshad; Belanger, David B.; Dai, Chaoyang; Li, Dansu; Girijavallabhan, Vinay M.; Popovici-Muller, Janeta; Yu, Wensheng; Zhao, Lianyun
PATENT ASSIGNEE(S): Schering Corporation, USA
SOURCE: PCT Int. Appl., 889 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005121130	A2	20051222	WO 2005-US19131	20050601

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-576153P P 20040602
OTHER SOURCE(S): MARPAT 144:69727
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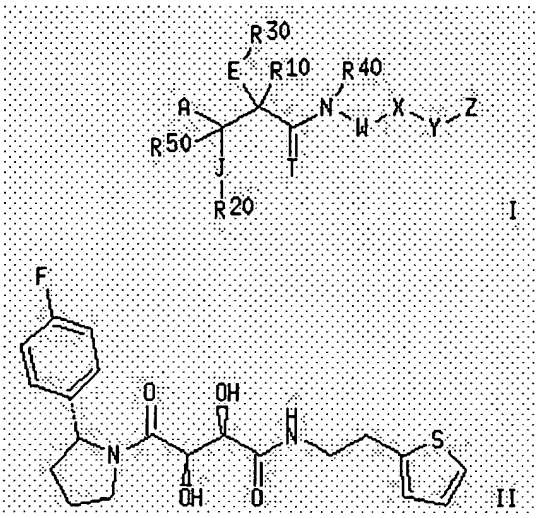

AB The title compds. I [A = (un)substituted benzimidazol-2-yl, imidazol-2-yl, CONH2, CSNH2; J, E = O, S, NR5 (wherein R5 = H, alkyl, alkylaryl); T = O, S; R10, R20 = H, alkyl, fluoroalkyl; R30 = H, alkyl or R30 and R40, taken together with N to which R40 is attached, are joined to form 4-7 membered (un)substituted heterocyclyl; R40, R50 = H, alkyl; W = [C(R13)2]n (wherein n = 0-5; R13 = H, halo, OH, etc.); X = a bond, alkyl, cycloalkyl, etc.; Y = a bond, O, S, NH, etc.; Z = H, alkyl, aryl, etc.; or their pharmaceutically acceptable salts] which can be useful for the treatment of diseases or conditions mediated by MMPs, ADAMs, TACE, TNF-α or combinations thereof, were prepd. E.g., a multi-step synthesis of II, starting from 2,2-dimethyl-[1,3]dioxolane-4R,5R-dicarboxylic acid monomethyl ester and 2-(thien-1-yl)ethylamine, was given. The compds. I were tested against TACE (biol. data given for representative compds. I).

IT **97483-77-7**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of tartaric acid functional compds. for the treatment of inflammatory disorders)

RN 97483-77-7 HCAPLUS

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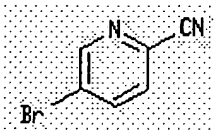

IT **173999-23-0P 871728-50-6P 871728-53-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of tartaric acid functional compds. for the treatment of inflammatory disorders)

RN 173999-23-0 HCAPLUS

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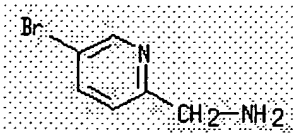

RN 871728-50-6 HCAPLUS

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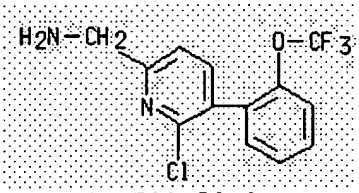

RN 871728-53-9 HCAPLUS
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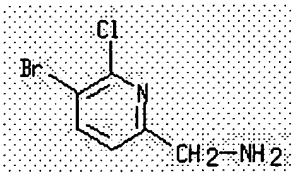

L11 ANSWER 3 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:1314348 HCAPLUS
DOCUMENT NUMBER: 144:51716
TITLE: Preparation of pyrroloquinoline and other phosphonate analogs of HIV-integrase inhibitors as anti-AIDS agents
INVENTOR(S): Cai, Zhenhong R.; Chen, Xiaowu; Fardis, Maria; Jabri, Salman Y.; Jin, Haolun; Kim, Choung U.; Metobo, Sanuel E.; Mish, Michael R.; Pastor, Richard M.
PATENT ASSIGNEE(S): Gilead Sciences, Inc., USA
SOURCE: PCT Int. Appl., 791 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005117904	A2	20051215	WO 2005-US12520	20050411

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-562678P P 20040414
OTHER SOURCE(S): MARPAT 144:51716
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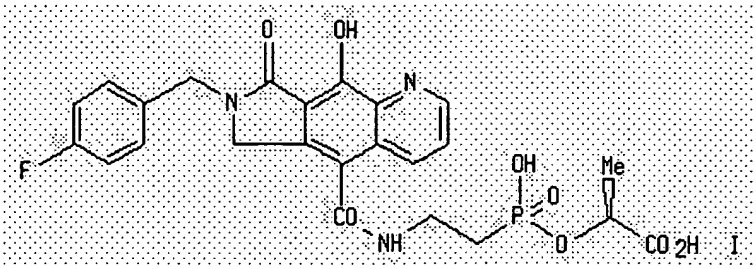

AB Novel HIV integrase inhibitor compds. having at least one phosphonate group (e.g. (S)-2-[[[2-[[[7-(4-fluorobenzyl)-9-hydroxy-8-oxo-7,8-dihydro-6H-pyrrolo[3,4-g]quinolin-5-yl]carbonyl]amino]ethyl](hydroxy)phosphinoyl]oxy]propionic acid (shown as I)), protected intermediates thereof, and methods for inhibition of HIV-integrase are disclosed. The inhibitors comprise ?1 covalently attached A0 groups [A0 = -[Y2[C(Ry)2]M12a]M12b-Y2-W6, -[Y2[C(Ry)2]M12a]M12b-Y2-W3 or -[Y2[C(Ry)2]M12a]M12b-P(:Y1)[Y2[P(:Y1)(Y2-Rx)Y2]M2-Rx]2]; ?1 A0 group is an A1 group. In the A0 groups: Y1 = O, S, NRx, N(O)(Rx), N(ORx), N(O)(ORx), or N(N(Rx)2); Y2 = a bond, O, NRx, N(O)(Rx), N(ORx), N(O)(ORx), N(N(Rx)2), S(O) (sulfoxide), S(O)2 (sulfone), S (sulfide), or S-S (disulfide); M2 is 0-2; M12a = 1-12; and M12b = 0-12; Ry = H, C1-C18 (un)substituted alkyl, C2-C18 (un)substituted alkenyl, C2-C18 (un)substituted alkynyl, C6-C20 (un)substituted aryl, or a protecting group, or where taken together at a C atom, two vicinal Ry groups form a carbocycle or a heterocycle; or taken together at a C atom, two vicinal Ry groups form a ring; such as, cyclopropyl, cyclobutyl, cyclopentyl, or cyclohexyl; or the ring may contain ?1 heteroatoms forming a heterocyclic ring such as, piperazinyl, piperidinyl, pyranyl, or tetrahydrofuryl. Rx = H, C1-C18 (un)substituted alkyl, C2-C18 (un)substituted alkenyl, C2-C18 (un)substituted alkynyl, C6-C20 (un)substituted aryl, a protecting group, or -[C(:Y1)Y2]M1a[C(Ry)2]M12c(Y2)M1c[C(:Y1)Y2]M1d-Ry; M1a, M1c, and M1d = 0 or 1, and M12c = 0-12; W3 is W4 or W5; W4 is R5, -C(Y1)R5, -C(Y1)W5, -SO2R5, or -SO2W5; W5 is a carbocycle or a heterocycle wherein W5 = substituted with 0 to 3 R2 groups; W3a is W4a or W5a; W4a is R5a, -C(Y1)R5a, -C(Y1)W5a, -SO2R5a, or -SO2W5a; W5a is a multivalent substituted carbocycle or heterocycle wherein W5a = substituted with 0 to 3 R2 groups; W6 is W3a independently substituted with 1, 2, or 3 A3 groups; addnl. details including provisos are given in the claims. They are nucleoside and non-nucleoside reverse transcriptase inhibitors, esp. HIV integrase inhibitors. For example, I was prepd. (60%) by base hydrolysis of the Et/Ph diester, which was prepd. by deprotection of the diphenylmethyl ether, which was prepd. by amide formation between (S)-2-[[(2-aminoethyl)(phenoxy)phosphinoyl]oxy]propionic acid Et ester (prepn. given) and 9-benzhydryloxy-7-(4-fluorobenzyl)-8-oxo-7,8-dihydro-6H-pyrrolo[3,4-g]quinoline-5-carboxylic acid (prepn. given) using HATU and DIEA in DMF. Certain compds. of the invention inhibited viral prodn., viral infectivity, or virus-induced cytopathic effect in HIV-infected MT-2 cells with EC50 < 10 μM and exhibited cytotoxicity toward uninfected MT-2 cells with CC50 < 10 μM. Thus, I, prodrugs of I, and their pharmaceutical compns. are useful as anti-AIDS agents, anti-infective agents, and immunomodulators (no data).

IT **33252-29-8P**, 6-Chloropyridine-2-carbonitrile **188637-75-4P** **312904-51-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of pyrroloquinoline and other phosphonate analogs of HIV-integrase inhibitors as anti-AIDS agents)

RN 33252-29-8 HCAPLUS

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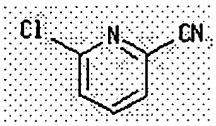

RN 188637-75-4 HCAPLUS
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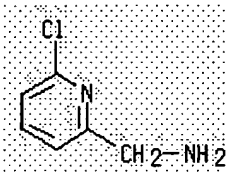

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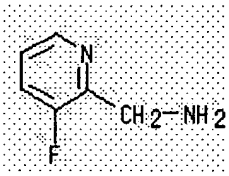

L11 ANSWER 4 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:1265299 HCAPLUS
DOCUMENT NUMBER: 144:22939
TITLE: Preparation of bicyclic heterocycles, particularly pyrimido[2,1-c][1,4]oxazine-2-carboxamides, as HIV integrase inhibitors
INVENTOR(S): Naidu, B. Narasimhulu; Banville, Jacques; Beaulieu, Francis; Connolly, Timothy P.; Krystal, Mark R.; Matiskella, John D.; Ouellet, Carl; Plamondon, Serge; Remillard, Roger; Sorenson, Margaret E.; Ueda, Yasutsugu; Walker, Michael A.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 156 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005267105	A1	20051201	US 2005-126891	20050511
WO 2005118593	A1	20051215	WO 2005-US16473	20050512

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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US 2005267131 A1 20051201 US 2005-138773 20050526
WO 2005118589 A1 20051215 WO 2005-US18567 20050527
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WO 2005118590 A1 20051215 WO 2005-US18568 20050527
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MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.:
US 2004-575513P P 20040528
US 2004-603371P P 20040820
US 2005-126891 A 20050511
US 2005-138726 A 20050526
US 2005-138773 A 20050526

OTHER SOURCE(S): MARPAT 144:22939

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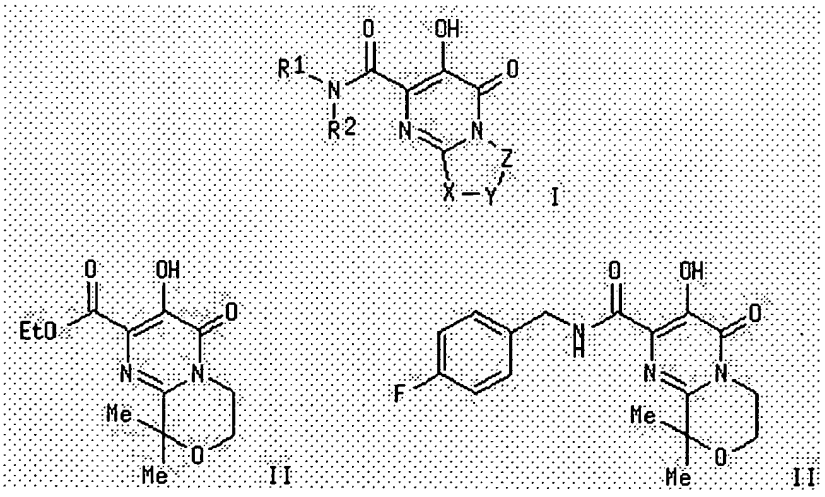
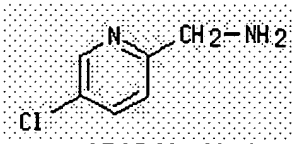


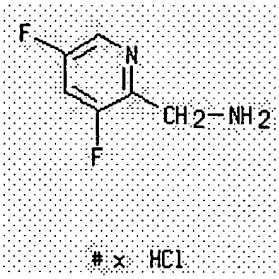
AB The invention is related to the prepn. of title compds. I [R1 = C1-6(Ar1)alkyl, C1-6(Ar1)oxyalkyl, C1-6(Ar1)hydroxyalkyl, etc.; R2 = H, alkyl, OH, alkyloxy; Ar1 = (un)substituted Ph, naphthyl, benzothiophenyl, etc.; X-Y-Z = C(R3)2OC(R3)2, C(R3)2OC(R3)2C(R3)2, C(R3)2C(R3)2C(R3)2C(R3)2; R3 = H, alkyl], and their pharmaceutically acceptable salts or solvates which inhibit HIV integrase and prevent viral integration into human DNA. The invention is also related to the pharmaceutical compns. comprising pyrimidinones I, and methods of using them for treating HIV infection and AIDS. Thus, reacting ester II (prepn. given) with 4-fluorobenzylamine in DMF/ethanol in the presence of TEA at 90? gave amide III in 82% yield. Selected I displayed IC50 values in the range of 0.002-0.1 μM for the inhibition of HIV integrase activity. II demonstrated synergistic or additive-synergistic HIV antiviral activity when used in combination with other antiviral agents, e.g., zidovudine, indinavir, T-20, etc.

IT **67938-76-5P**, (5-Chloropyridin-2-yl)methanamine
870562-68-8P, (3,5-Difluoropyridin-2-yl)methanamine hydrochloride
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of bicyclic heterocycles as HIV integrase inhibitors)

RN 67938-76-5 HCAPLUS
CN 2-Pyridinemethanamine, 5-chloro- (9CI) (CA INDEX NAME)

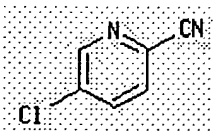


RN 870562-68-8 HCAPLUS
CN 2-Pyridinemethanamine, 3,5-difluoro-, hydrochloride (9CI) (CA INDEX NAME)

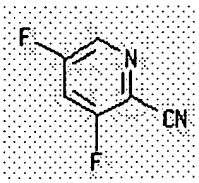


IT **89809-64-3** **298709-29-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of bicyclic heterocycles as HIV integrase inhibitors)

RN 89809-64-3 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-chloro- (9CI) (CA INDEX NAME)



RN 298709-29-2 HCAPLUS
CN 2-Pyridinecarbonitrile, 3,5-difluoro- (9CI) (CA INDEX NAME)



L11 ANSWER 5 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:1042217 HCAPLUS
DOCUMENT NUMBER: 143:325976
TITLE: Diaminoalcohols as renin inhibitors, their preparation and pharmaceutical compositions
INVENTOR(S): Herold, Peter; Stutz, Stefan; Mah, Robert; Tschinke, Vincenzo; Stojanovic, Aleksandar; Jotterand, Nathalie; Quirmbach, Michael; Behnke, Dirk; Marti, Christiane
PATENT ASSIGNEE(S): Speedel Experimenta A.-G., Switz.
SOURCE: PCT Int. Appl., 88 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005090304	A1	20050929	WO 2005-EP51241	20050317

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

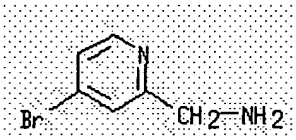
PRIORITY APPLN. INFO.: CH 2004-479 A 20040319
OTHER SOURCE(S): MARPAT 143:325976
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

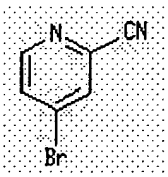
AB The invention relates to diaminoalcs. I, which are renin inhibitors. In compds. I, X is methylene or hydroxymethylene; R1 is H, (un)substituted C1-8 alkyl, (un)substituted C3-8 cycloalkyl, (un)substituted C1-8 alkanoyl, (un)substituted C1-8 alkoxycarbonyl, aryl-C0-4alkyl, or heterocyclyl-C0-4alkyl; R2 is (un)substituted C1-8 alkyl, (un)substituted C3-8 cycloalkyl, (un)substituted C1-8 alkanoyl, etc., or R1 and R2, together with the nitrogen atom to which they are bonded, form a satd. or partly unsatd. 4- to 8-membered heterocyclic ring; R3 and R4 are independently selected from H, C1-4 alkyl, C1-8 alkoxycarbonyl, and C1-8 alkanoyl; R5 are independently selected from H, C1-8 alkyl, or together with the carbon atom to which they are bonded, form a C3-8 cycloalkylene; and R6 is (un)substituted heterocyclyl or (un)substituted polycyclic,

unsatd. hydrocarbon; including salts or prodrugs thereof, or in which one or more atoms have been replaced by their stable, non-radioactive isotopes. The invention also relates to the prepn. of I, pharmaceutical compns. contg. compd. I as an active pharmaceutical ingredient, in free form or as a pharmaceutically usable salt, as well as to the use of the compns. as renin inhibitors, including in combination with other pharmaceutical agents. Substitution of 1-bromo-2-methoxyethane with Me 8-hydroxynaphthalene-2-carboxylate followed by hydride redn., bromination, and substitution with (R)-4-benzyl-3-(3-methylbutyryl)oxazolidin-2-one resulted in the formation of II. Cleavage of the chiral auxiliary from II, borane redn., bromination, substitution with 3,6-diethoxy-2,5-dihydropyrazine, hydrolysis, and N-protection gave amino acid III. The ester functionality of III was reduced to the alc., followed by oxidn. to the aldehyde, epoxidn. with trimethylsulfoxonium iodide, ring opening with piperidine, and deprotection to give the dihydrochloride of diaminoalc. IV. The compds. of the invention act as renin inhibitors (no data).

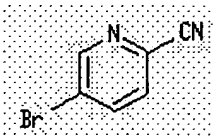
IT **865156-50-9P**, [(4-Bromopyridin-2-yl)methyl]amine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of diaminoalcs. as renin inhibitors)
RN 865156-50-9 HCAPLUS
CN 2-Pyridinemethanamine, 4-bromo- (9CI) (CA INDEX NAME)



IT **62150-45-2**, 4-Bromopyridine-2-carbonitrile **97483-77-7**, 5-Bromopyridine-2-carbonitrile
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(starting material; prepn. of diaminoalcs. as renin inhibitors)
RN 62150-45-2 HCAPLUS
CN 2-Pyridinecarbonitrile, 4-bromo- (9CI) (CA INDEX NAME)



RN 97483-77-7 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-bromo- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 6 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:979618 HCAPLUS
DOCUMENT NUMBER: 143:286301
TITLE: Preparation of 6-substituted 2,3,4,5-tetrahydro-1H-benzo[d]azepines as 5-HT2c receptor agonists

INVENTOR(S): Allen, John Gordon; Briner, Karin; Cohen, Michael Philip; Galka, Christopher Stanley; Hellman, Sarah Lynne; Martinez-Grau, Maria Angeles; Reinhard, Matthew Robert; Rodriguez, Michael John; Rothhaar, Roger Ryan; Tidwell, Michael Wade; Victor, Frantz; Williams, Andrew Caerwyn; Zhang, Deyi; Boyd, Steven Armen; Conway, Richard Gerard; Deo, Arundhati S.; Lee, Wai-Man; Siedem, Christopher Stephen; Singh, Ajay

PATENT ASSIGNEE(S): Eli Lilly and Company, USA

SOURCE: PCT Int. Appl., 595 pp.
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005082859	A1	20050909	WO 2005-US5418	20050218

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2004-547681P P 20040225

OTHER SOURCE(S): MARPAT 143:286301

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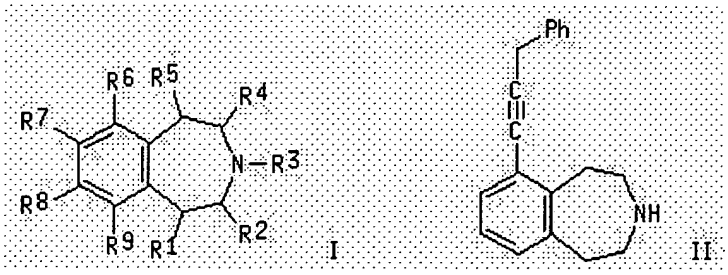
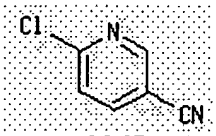
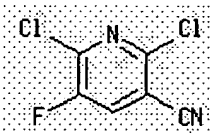


AB The title compds. I [R1 = H, F, alkyl; R2-R4 = H, Me, Et; R5 = H, F, Me, Et; R6 = C?CR10, OR12, SR14, substituted NH2; R7 = H, halo, CN, etc.; R8 = H, halo, CN, SCF3; R9 = H, halo, CN, etc.; R10 = CF3, alkyl, fluoroalkyl, etc.; R12 = pyridylalkyl, thiazolylalkyl, etc.; R13 = cycloalkylalkyl, alkoxy, fluoroalkoxy, etc.; R14 = tetrahydropyranyl, tetrahydrofuranyl, etc.], useful as selective 5-HT2c receptor agonists for the treatment of 5-HT2c assocd. disorders including obesity, obsessive/compulsive disorder, depression, and anxiety, were prepd. Thus, reacting 3-tert-butoxycarbonyl-6-trifluoromethanesulfonyloxy-2,3,4,5-tetrahydro-1H-benzo[d]azepine (prepn. given) with 3-phenyl-1-propyne followed by deprotection afforded 85% II.HCl. Representative compds. I are found to have excellent affinity for the 5-HT2c receptor, with Ki's typically less than or equal to about 200 nM.

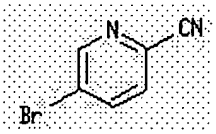
IT **33252-28-7** **82671-02-1** **97483-77-7**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of 6-substituted 2,3,4,5-tetrahydro-1H-benzo[d]azepines as 5-HT2c receptor agonists)
RN 33252-28-7 HCAPLUS
CN 3-Pyridinecarbonitrile, 6-chloro- (9CI) (CA INDEX NAME)



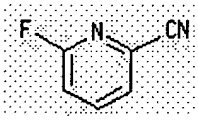
RN 82671-02-1 HCAPLUS
CN 3-Pyridinecarbonitrile, 2,6-dichloro-5-fluoro- (9CI) (CA INDEX NAME)



RN 97483-77-7 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-bromo- (9CI) (CA INDEX NAME)



IT **3939-15-9P** **89809-64-3P** **97509-75-6P**
205744-18-9P **312904-49-7P** **327056-62-2P**
561297-96-9P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 6-substituted 2,3,4,5-tetrahydro-1H-benzo[d]azepines as 5-HT2c receptor agonists)
RN 3939-15-9 HCAPLUS
CN 2-Pyridinecarbonitrile, 6-fluoro- (9CI) (CA INDEX NAME)



RN 89809-64-3 HCAPLUS
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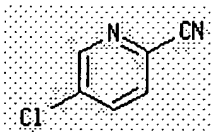

RN 97509-75-6 HCAPLUS
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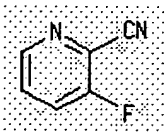

RN 205744-18-9 HCAPLUS
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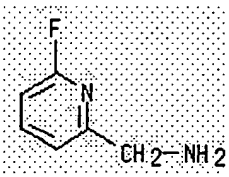

RN 312904-49-7 HCAPLUS
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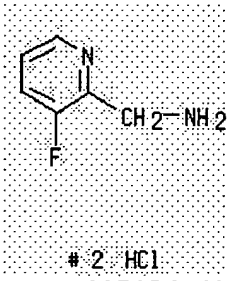
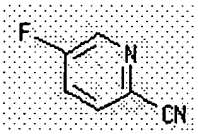


RN 327056-62-2 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-fluoro- (9CI) (CA INDEX NAME)



RN 561297-96-9 HCAPLUS
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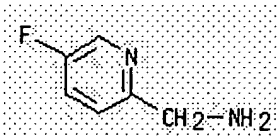


REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 7 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:638844 HCAPLUS
DOCUMENT NUMBER: 143:133274
TITLE: Preparation of arylsulfonyl-substituted indoles as CB1 receptor modulators
INVENTOR(S): Allen, Jennifer Rebecca; Amegadzie, Albert Kudzovi; Gardinier, Kevin Matthew; Gregory, George Stuart; Hitchcock, Steven Andrew; Hoogestraat, Paul J.; Jones, Winton Dennis, Jr.; Smith, Daryl Lynn
PATENT ASSIGNEE(S): Eli Lilly and Company, USA
SOURCE: PCT Int. Appl., 204 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005066126	A1	20050721	WO 2004-US39763	20041213

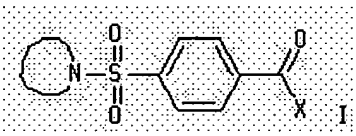
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW

RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-532247P P 20031223

OTHER SOURCE(S): MARPAT 143:133274

GI

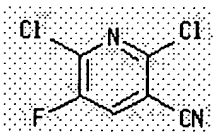


AB Title compds. I [the nitrogen contg. ring = indolyl, pyrrolopyridinyl, etc.; X = amino, etc.] are prepd. For instance,. N-(4-Fluorobenzyl)-4-[(3-phenylpyrrolo[3,2-c]pyridine-1-yl)sulfonyl]benzamide is prepd. from 3-Phenyl-1H-pyrrolo[3,2-c]pyridine (prepn. given) and 4-(4-Fluorobenzylcarbamoyl)benzenesulfonyl chloride (THF, KOBu-t, 16 h). Compds. of the invention exhibit IC50 ? 5 μM for the CB1 and CB2 receptors. I are useful in the treatment of psychosis, memory deficits, cognitive disorders, migraine, neuropathy, neuro-inflammatory disorders (e.g., multiple sclerosis, Guillain-Barre syndrome and the inflammatory sequelae of viral encephalitis), cerebral vascular accidents, head trauma, anxiety disorders, stress, epilepsy, Parkinson's disease and schizophrenia. I are also useful for the treatment of substance abuse disorders, particularly to opiates, alc., and nicotine and for the treatment of obesity or eating disorders assocd. with excessive food intake and complications assocd. therewith.

IT **82671-02-1**, 2,6-Dichloro-3-cyano-5-fluoropyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of arylsulfonyl-substituted indoles as CB1 receptor modulators)

RN 82671-02-1 HCAPLUS

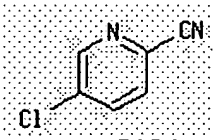
CN 3-Pyridinecarbonitrile, 2,6-dichloro-5-fluoro- (9CI) (CA INDEX NAME)



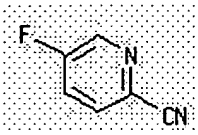
IT **89809-64-3P**, 5-Chloro-2-cyanopyridine **327056-62-2P**, 2-Cyano-5-fluoropyridine **859164-78-6P**, 2-Aminomethyl-5-fluoropyridine dihydrochloride
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of arylsulfonyl-substituted indoles as CB1 receptor modulators)

RN 89809-64-3 HCAPLUS

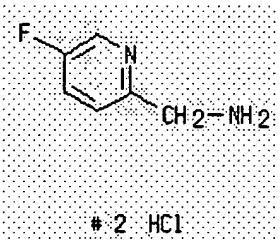
CN 2-Pyridinecarbonitrile, 5-chloro- (9CI) (CA INDEX NAME)



RN 327056-62-2 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-fluoro- (9CI) (CA INDEX NAME)



RN 859164-78-6 HCAPLUS
CN 2-Pyridinemethanamine, 5-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 8 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2005:612238 HCAPLUS
DOCUMENT NUMBER: 143:133188
TITLE: Preparation of α-hydroxy carboxamides, particularly N-biphenylmethyl and N-phenylpyridin-2-ylmethyl amides, as bradykinin B1 antagonists or inverse agonists useful in the treatment of pain and inflammation
INVENTOR(S): Wood, Michael R.; Anthony, Neville J.; Bock, Mark G.; Kuduk, Scott D.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 51 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2005063690	A1	20050714	WO 2004-US42691	20041217

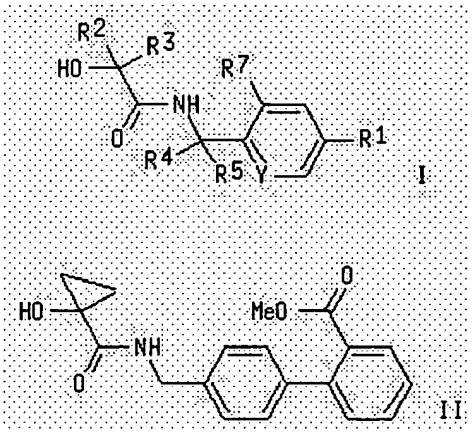
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,

AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2003-531643P P 20031222
US 2004-539637P P 20040128
US 2004-624958P P 20041104

OTHER SOURCE(S): MARPAT 143:133188

GI

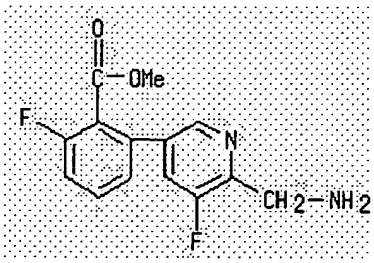


AB Title compds. [I; Y = CH, N; R1 = (un)substituted Ph, 2,2-dioxo-2,1-benzisothiazolin-1-yl; R2 = H, (un)substituted alkyl, Ph, etc.; R3 = defined as R2; or R3 = OH; or R2CR3 = (un)substituted 3-7-membered carbocyclyl; R4, R5 = independently H, halo/alkyl; R7 = H, halo] were prepd. as bradykinin B1 antagonists or inverse agonists useful in the treatment of pain and inflammation assocd. with the bradykinin B1 pathway. For example, coupling of 1-hydroxycyclopropanecarboxylic acid with Me 4'-(aminomethyl)biphenyl-2-carboxylate gave amide II. I have affinity for the B1 receptor in a radioligand assay as demonstrated by results of less than 5 μM [sic].

IT **858414-19-4P**, Methyl 2-[6-(aminomethyl)-5-fluoropyridin-3-yl]-6-fluorobenzoate
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of α-hydroxy N-biphenylmethyl and N-phenylpyridin-2-ylmethyl amides as bradykinin B1 antagonists or inverse agonists useful in the treatment of pain and inflammation)

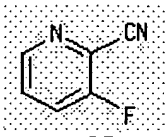
RN 858414-19-4 HCAPLUS

CN Benzoic acid, 2-[6-(aminomethyl)-5-fluoro-3-pyridinyl]-6-fluoro-, methyl ester (9CI) (CA INDEX NAME)

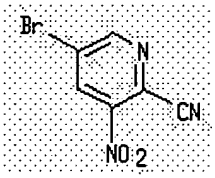


IT **97509-75-6**, 2-Cyano-3-fluoropyridine **573675-25-9**,

5-Bromo-3-nitropyridine-2-carbonitrile
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of α-hydroxy N-biphenylmethyl and N-phenylpyridin-2-ylmethyl amides as bradykinin B1 antagonists or inverse agonists useful in the treatment of pain and inflammation)
RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



RN 573675-25-9 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-bromo-3-nitro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

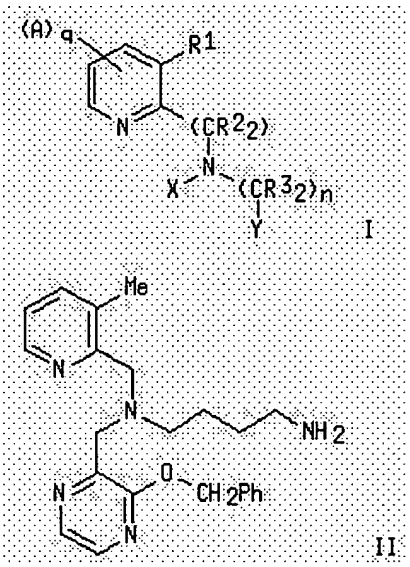
L11 ANSWER 9 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN
Full Text | Citing References

ACCESSION NUMBER: 2004:878165 HCAPLUS
DOCUMENT NUMBER: 141:379809
TITLE: Preparation of pyridine derivatives as CXCR4 chemokine receptor binding compounds
INVENTOR(S): Bridger, Gary; McEachern, Ernest J.; Skerlj, Renato; Schols, Dominique
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 211 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004209921	A1	20041021	US 2004-823494	20040412
CA 2520259	AA	20041028	CA 2004-2520259	20040412
WO 2004091518	A2	20041028	WO 2004-US11328	20040412
WO 2004091518	A3	20041223		

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

EP 1613613 A2 20060111 EP 2004-759481 20040412
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR
PRIORITY APPLN. INFO.: US 2003-462736P P 20030411
US 2003-505688P P 20030923
WO 2004-US11328 W 20040412
OTHER SOURCE(S): MARPAT 141:379809
GI

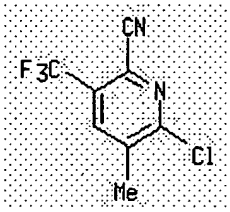


AB Title compds. I [X = (CR32)o-(CR3=CR3)p-(CR32)r-NR52, (CR32)s-R4, (un)substituted mono or bicyclic ring optionally contg. N, O or S, etc.; Y = (un)substituted N-contg. monocyclic or bicyclic arom. or partially arom. moiety; A and R1 = non-interfering substituent provided that two As do not form a ring; R2 and R3 = H or (un)substituted alkyl; R4 = (un)substituted heterocycle or a hetero compd.; R5 = H or alkyl; wherein R1 and R2 is not H; and wherein R1 and R2 may be connected to form an addnl. ring if Y does not contain a 2-imidazoyl residue optionally connected to an addnl. ring; q and n independently = 0-4; p = 0-1; o and r independently = 1-4; s = 1-6 provided that if X = (CR3)2-R4, r is at least two if R4 = 2-pyridinyl, quinolinyl, imidazolyl or furan], as well as their pharmaceutically acceptable salts, are prepd. and disclosed as having the ability to bind to chemokine receptors, in particular CXCR4. Thus, e.g., II was prepd. by reductive amination of {4-[(3-methylpyridin-2-ylmethyl)-amino]-butyl}carbamic acid tert-Bu ester (prepn. given) with 3-benzyloxypyrazine-2-carbaldehyde. The present invention also relates to methods of using such compds., such as in treating HIV infection and inflammatory conditions such as rheumatoid arthritis. In assays to evaluate inhibition of HIV-1, many compds. of the invention exhibited IC50 values in the range of 0.5nM-5μM. Furthermore, the present invention relates to methods to elevate progenitor and stem cell counts, as well as methods to elevate white blood cell counts, using such compds.

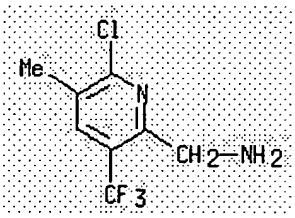
IT 780802-39-3P 780802-40-6P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of pyridine derivs. as CXCR4 chemokine receptor binding compds.)

RN 780802-39-3 HCAPLUS

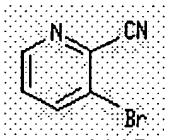
CN 2-Pyridinecarbonitrile, 6-chloro-5-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



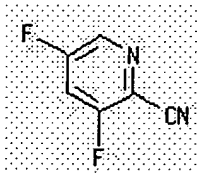
RN 780802-40-6 HCAPLUS
CN 2-Pyridinemethanamine, 6-chloro-5-methyl-3-(trifluoromethyl)- (9CI) (CA INDEX NAME)



IT **55758-02-6 298709-29-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(starting material; prepn. of pyridine derivs. as CXCR4 chemokine receptor binding compds.)
RN 55758-02-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-bromo- (9CI) (CA INDEX NAME)



RN 298709-29-2 HCAPLUS
CN 2-Pyridinecarbonitrile, 3,5-difluoro- (9CI) (CA INDEX NAME)



L11 ANSWER 10 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2004:203618 HCAPLUS
DOCUMENT NUMBER: 140:253570
TITLE: Preparation of N-biarylmethylaminocycloalkanecarboxamide as bradykinin B1 antagonists
INVENTOR(S): Kuduk, Scott D.; Wood, Michael R.; Bock, Mark G.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 59 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004019868	A2	20040311	WO 2003-US26628	20030825
WO 2004019868	A3	20040429		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2495914	AA	20040311	CA 2003-2495914	20030825
BR 2003013239	A	20050614	BR 2003-13239	20030825
EP 1545538	A2	20050629	EP 2003-791763	20030825
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2005537323	T2	20051208	JP 2004-532994	20030825
US 2005288305	A1	20051229	US 2005-523911	20050208
NO 2005001539	A	20050525	NO 2005-1539	20050323
PRIORITY APPLN. INFO.:			US 2002-406742P P	20020829
			WO 2003-US26628 W	20030825

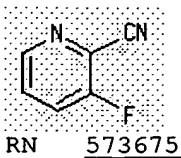
OTHER SOURCE(S): MARPAT 140:253570
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

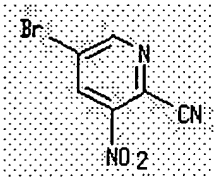
AB Title compds. I [Het = pyridyl, pyrimidinyl, N-oxide thereof; R1-2 = H, alkyl; R3a-3b = H, alkyl; R4a-4b = H, halo, alkyl, etc.; R5 = alkyl, cycloalkyl, alkynyl, alkenyl, etc.; R6a = alkyl, cycloalkyl, alkenyl, etc.; R6b-6c = H and not more than one of R6a-6c = heterocycle; R7a-7b = H, halo, CN, etc.; m = 0-3] are prepd. For instance, 1-[((pyrimidin-5-yl)carbonyl)amino]cyclobutanecarboxylic acid (prepn. given) is coupled to Me 2-[2-(aminomethyl)pyrimidin-5-yl]-6-fluorobenzoate (prepn. given; DMF, HOBt, EDCI, Et3N) to give II. Compds. of the invention have affinity for the bradykinin B1 receptor at less than 5 μM. I are useful for the treatment of pain and inflammation.

IT **97509-75-6**, 2-Cyano-3-fluoropyridine **573675-25-9**, 5-Bromo-3-nitropyridine-2-carbonitrile
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of N-biarylmethylaminocycloalkanecarboxamide as bradykinin B1 antagonists)

RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)

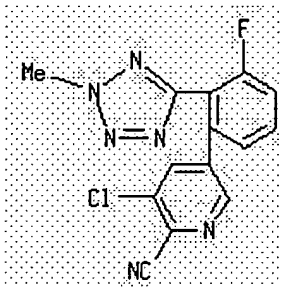


RN 573675-25-9 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-bromo-3-nitro- (9CI) (CA INDEX NAME)

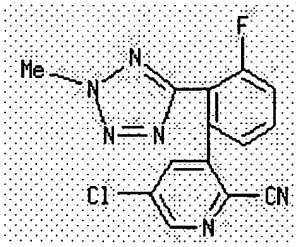


IT **669066-28-8P**, 3-Chloro-5-[3-fluoro-2-(2-methyl-2H-tetrazol-5-yl)phenyl]pyridine-2-carbonitrile **669066-30-2P**, 5-Chloro-3-[3-fluoro-2-(2-methyl-2H-tetrazol-5-yl)phenyl]pyridine-2-carbonitrile **669066-31-3P**, 1-[3-Chloro-5-[3-fluoro-2-(2-methyl-2H-tetrazol-5-yl)phenyl]pyridin-2-yl]methanamine **669066-35-7P**, 3-Fluoro-4-iodopyridine-2-carbonitrile **669066-36-8P**, 3-Fluoro-5-iodopyridine-2-carbonitrile **669066-37-9P**, Methyl 2-(6-cyano-5-fluoropyridin-3-yl)-6-fluorobenzoate
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of N-biarylmethylaminocycloalkanecarboxamide as bradykinin B1 antagonists)

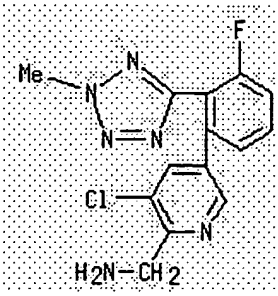
RN 669066-28-8 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-chloro-5-[3-fluoro-2-(2-methyl-2H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)



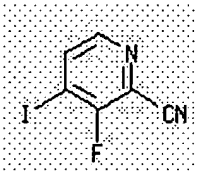
RN 669066-30-2 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-chloro-3-[3-fluoro-2-(2-methyl-2H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)



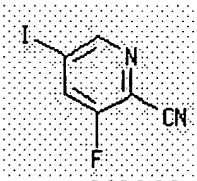
RN 669066-31-3 HCAPLUS
CN 2-Pyridinemethanamine, 3-chloro-5-[3-fluoro-2-(2-methyl-2H-tetrazol-5-yl)phenyl]- (9CI) (CA INDEX NAME)



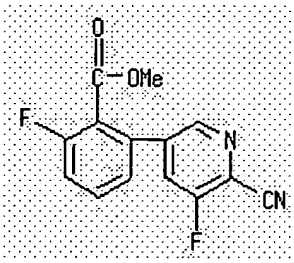
RN 669066-35-7 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro-4-iodo- (9CI) (CA INDEX NAME)



RN 669066-36-8 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro-5-iodo- (9CI) (CA INDEX NAME)



RN 669066-37-9 HCAPLUS
CN Benzoic acid, 2-(6-cyano-5-fluoro-3-pyridinyl)-6-fluoro-, methyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 11 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

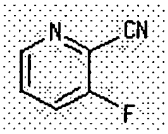
Full Text | Citing References

ACCESSION NUMBER: 2004:85763 HCAPLUS
DOCUMENT NUMBER: 140:272675
TITLE: Development of a Scaleable Synthesis of a 3-Aminopyrazinone Acetamide Thrombin Inhibitor
AUTHOR(S): Ashwood, Michael S.; Alabaster, Ramon J.; Cottrell, Ian F.; Cowden, Cameron J.; Davies, Antony J.; Dolling, Ulf H.; Emerson, Khateeta M.; Gibb, Andrew D.; Hands, David; Wallace, Debra J.; Wilson, Robert D.
CORPORATE SOURCE: Department of Process Research, Merck Sharp and Dohme Research Laboratories, Hoddesdon, Hertfordshire, EN11 9BU, UK
SOURCE: Organic Process Research & Development (2004), 8(2), 192-200
CODEN: OPRDFK; ISSN: 1083-6160

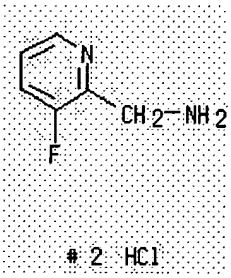
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:272675

AB A scaleable route to 2-{3-[(2,2-difluoro-2-(2-pyridyl)ethyl)amino]-6-chloro-2-oxohydropyrazinyl}-N-[(3-fluoro(2-pyridyl))methyl]acetamide (I) is described in which various scaleup issues were addressed to provide a safe, efficient, and robust route for the prepn. of multi-kilo amts. of the compd. The use of expensive and toxic reagents, notably sodium azide, TMS-cyanide, and Deoxo-Fluor, and the need for specialist equipment were overcome in the prepn. of the key fluorinated intermediates 2,2-difluoro-2-(2-pyridyl)ethylamine and 2-aminomethyl-3-fluoropyridine. With minimal isolations and through processing of intermediates, the thrombin inhibitor I was isolated in 36% overall yield.

IT **97509-75-6P**, 3-Fluoropyridine-2-carbonitrile
RL: IMF (Industrial manufacture); **RCT (Reactant)**; PREP (Preparation); RACT (Reactant or reagent)
(intermediate; scaleup synthesis route with min. steps and safer reagents for 3-aminopyrazinone acetamide thrombin inhibitor)
RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



IT **312904-49-7P**, 2-Aminomethyl-3-fluoropyridine dihydrochloride
RL: IMF (Industrial manufacture); PUR (Purification or recovery); RCT (Reactant); **PREP (Preparation)**; RACT (Reactant or reagent)
(recrystd., intermediate; scaleup synthesis route with min. steps and safer reagents for 3-aminopyrazinone acetamide thrombin inhibitor)
RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 12 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Chng References

ACCESSION NUMBER: 2003:913147 HCAPLUS
DOCUMENT NUMBER: 139:381477
TITLE: Preparation of 4,5-dihydro-1H-benzo[g]indazole-3-carboxamides as IKK2 inhibitors for the treatment of cancer and inflammation
INVENTOR(S): Lennon, Patrick; Bonafoux, Dominique; Oburn, David S.; Wolfson, Serge G.
PATENT ASSIGNEE(S): Pharmacia Corporation, USA
SOURCE: PCT Int. Appl., 312 pp.

CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003095430	A1	20031120	WO 2003-US8917		20030319
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
WO 2003024935	A2	20030327	WO 2002-US29774		20020919
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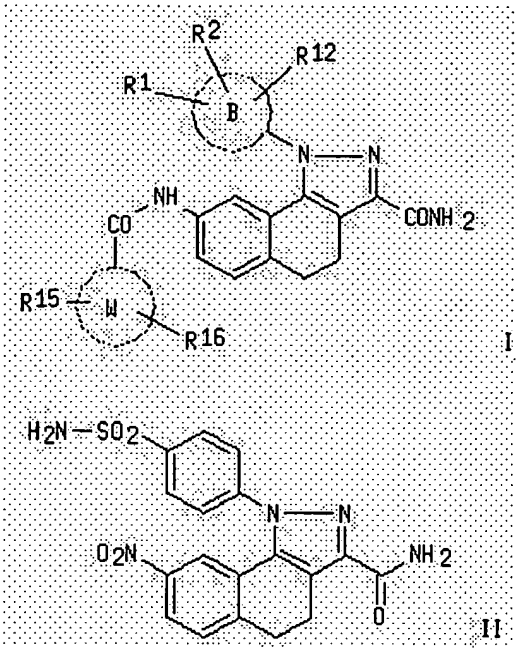
CA 2485298	AA	20031120	CA 2003-2485298		20030319
EP 1501805	A1	20050202	EP 2003-716793		20030319
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK					
BR 2003010010	A	20050215	BR 2003-10010		20030319
JP 2005530773	T2	20051013	JP 2004-503448		20030319
US 2005256180	A1	20051117	US 2005-113926		20050425
PRIORITY APPLN. INFO.:			US 2002-379090P	P	20020509
			WO 2002-US29774	A	20020919
			US 2001-323423P	P	20010919
			US 2002-247096	A3	20020919
			WO 2003-US8917	W	20030319

OTHER SOURCE(S): MARPAT 139:381477
GI

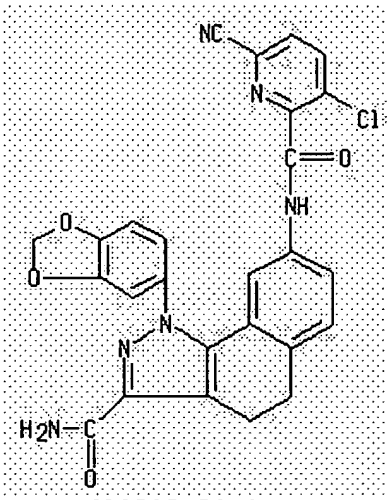


AB The present invention relates to substituted pyrazolyl derivs., compns. comprising such, intermediates, methods of making substituted pyrazolyl derivs., and methods for treating cancer, inflammation, and inflammation-assocd. disorders, such as arthritis. 4,5-Dihydro-1H-benzo[g]indazole-3-carboxamides (shown as I; variables defined below; e.g. II) were prepd. via conventional and solid phase synthetic methods as IκB protein kinase β (IKKβ or IKK2) inhibitors. Although the methods of prepn. are not claimed, 480 example prepns. and/or characterization data are included. For example, reaction of 7-nitro-1-tetralone with Et acetate in the presence of Li bis(trimethylsilyl)amide in ether gave the 1,3-diketone (87%), which was cyclized with 4-sulfonamidophenylhydrazine?HCl with HCl in MeOH to give the Et 1H-dihydrobenzo[g]indazolecarboxylate (69%). Amidation with NH4OH in MeOH provided II. In IKKβ resin enzyme assays, I exhibited IKKβ activity with IC50 values ranging from ? 1 μM to > 100 μM. Thus, I are useful for treating cancer, inflammation, and inflammation-assocd. disorders, such as arthritis (no data). For I: B is a 5 or 6 membered heteroaryl, aryl, (un)satd. heterocyclic (un)substituted with R1, R2, and R12; W is a 5 or 6 membered heteroaryl, aryl, (un)satd. heterocyclic. R1 = hydrido, halo, alkyl, aryl, heteroaryl, alkenyl, alkynyl, haloalkyl, CN, NO2, OR5, OCOOR5, CO2R7, CON(R6)R7, COR6, SR6, SOR6, SO2R6, NR6R7, NR6COR7, NR6CONHR7, NR6SO2R7, NR6SO2NHR7, and SO2N(R6)R7; R2 = halo, hydrido, hydroxyalkyl, alkyl, OR6, CN, NO2, SR6, NHR6, CON(R6)R7, NHCONHR6, CO2H, and haloalkyl; R1 and R2 may be taken together to form a 5 to 7 membered (un)satd. carbocyclic ring optionally contg. 0 to 3 heteroatoms N, O, or S, and wherein said ring is (un)substituted with R1. R12 = hydrido, halo, alkyl, and alkoxy; R15 = alkylsulfonamide, sulfamyl, alkyl, alkylthio, alkylsulfinyl, alkylsulfonyl, alkylamino, aminoalkyl, alkylaminoalkyl, dialkylaminoalkyl, alkoxy, halo, acyloxy, oxy, formyl, haloalkyl, cyano, haloalkoxy, acyl, carboxy, hydroxy, hydroxyalkyloxy, phenoxy, nitro, azido, benzyloxy, dialkylaminoacyl, thioalkyl, aminoacyloxy, thiocyanate, isothiocyanate, alkyldioxy, hydroxyalkyl, alkylamino, alkyloxycarbonyl, alkoxyalkyl, alkenylamino, alkynylamino, alkenyl, alkynyl, dialkylaminoalkyloxy, and heterocyclic; addnl. details are given in the claims.

IT **623585-57-9P**, 1-(1,3-Benzodioxol-5-yl)-8-[[(3-chloro-6-cyanopyridin-2-yl)carbonyl]amino]-4,5-dihydro-1H-benzo[g]indazole-3-

carboxamide **623585-58-0P** **623585-62-6P**
623585-64-8P, 1-(1,3-Benzodioxol-5-yl)-8-[(5-chloro-2-cyanoisonicotinoyl)amino]-4,5-dihydro-1H-benzo[g]indazole-3-carboxamide
623585-66-0P
RL: PAC (Pharmacological activity); **RCT (Reactant)**; SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; RACT (Reactant or reagent); USES (Uses)
(drug candidate; prepn. of 4,5-dihydro-1H-benzo[g]indazole-3-carboxamides as IKK2 inhibitors for treatment of cancer and inflammation)

RN 623585-57-9 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 1-(1,3-benzodioxol-5-yl)-8-[[(3-chloro-6-cyano-2-pyridinyl)carbonyl]amino]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 623585-58-0 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[6-(aminomethyl)-3-chloro-2-pyridinyl]carbonyl]amino]-1-(1,3-benzodioxol-5-yl)-4,5-dihydro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 623585-56-8
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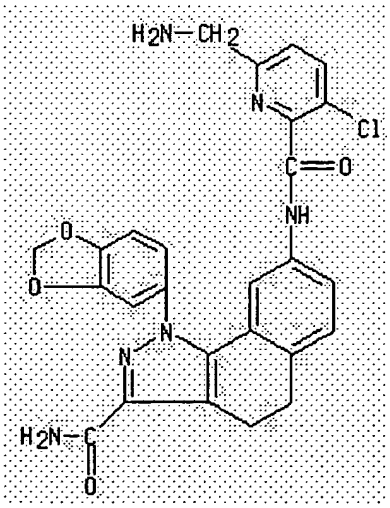

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CRN 76-05-1
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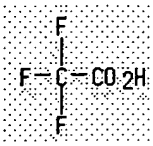

RN 623585-62-6 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[2-(aminomethyl)-5-chloro-4-pyridinyl]carbonyl]amino]-1-(4-fluorophenyl)-4,5-dihydro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 623585-61-5
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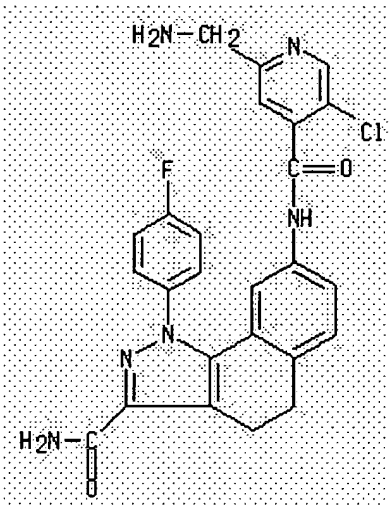

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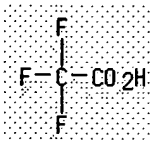
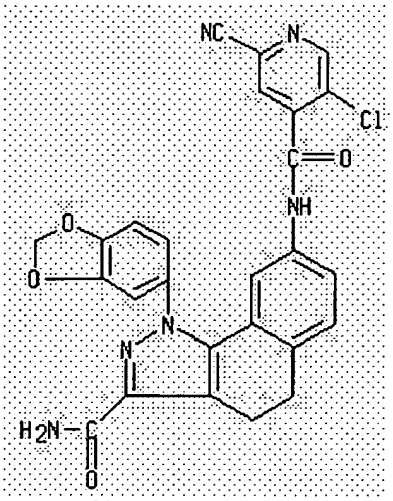


RN 623585-64-8 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 1-(1,3-benzodioxol-5-yl)-8-[[(5-chloro-2-cyano-4-pyridinyl)carbonyl]amino]-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 623585-66-0 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[2-(aminomethyl)-5-chloro-4-pyridinyl]carbonyl]amino]-1-(1,3-benzodioxol-5-yl)-4,5-dihydro-, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

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CRN 623585-65-9
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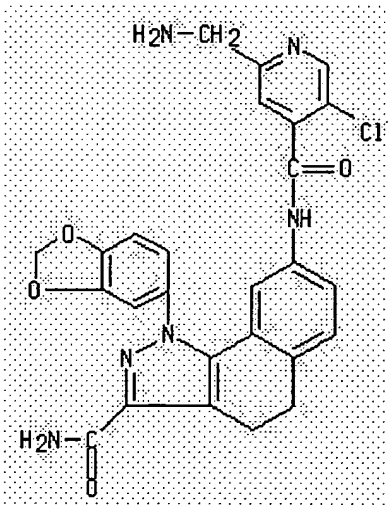
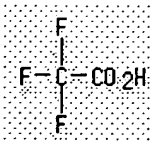


CM 2

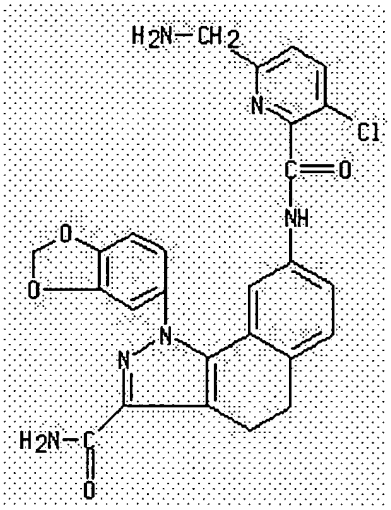
CRN 76-05-1
CMF C2 H F3 O2



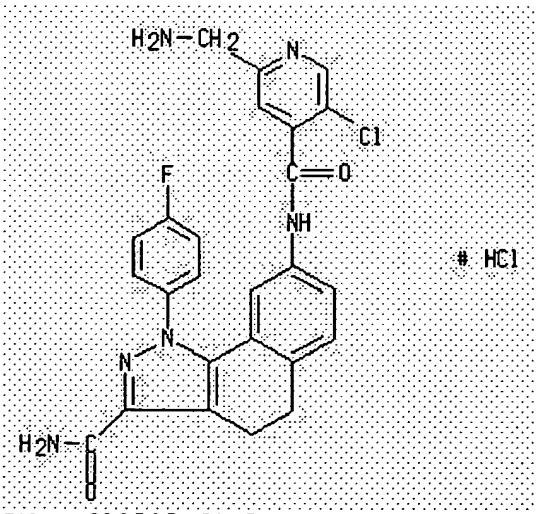
IT **623585-56-8P**, 8-[[[6-(Aminomethyl)-3-chloropyridin-2-yl]carbonyl]amino]-1-(1,3-benzodioxol-5-yl)-4,5-dihydro-1H-benzo[g]indazole-3-carboxamide **623585-60-4P** **623585-61-5P**, 8-[[2-(Aminomethyl)-5-chloroisonicotinoyl]amino]-1-(4-fluorophenyl)-4,5-dihydro-1H-benzo[g]indazole-3-carboxamide **623585-63-7P**

623585-65-9P, 8-[[2-(Aminomethyl)-5-chloroisonicotinoyl]amino]-1-(1,3-benzodioxol-5-yl)-4,5-dihydro-1H-benzo[g]indazole-3-carboxamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(drug candidate; prepn. of 4,5-dihydro-1H-benzo[g]indazole-3-carboxamides as IKK2 inhibitors for treatment of cancer and inflammation)

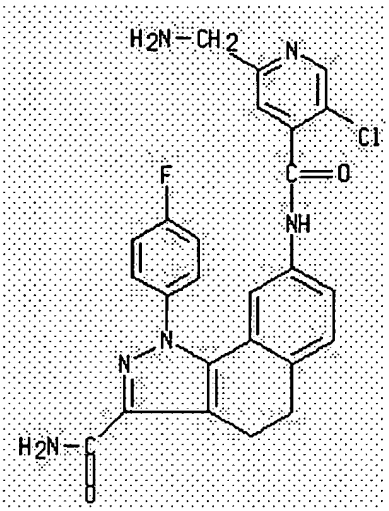
RN 623585-56-8 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[6-(aminomethyl)-3-chloro-2-pyridinyl]carbonyl]amino]-1-(1,3-benzodioxol-5-yl)-4,5-dihydro- (9CI) (CA INDEX NAME)



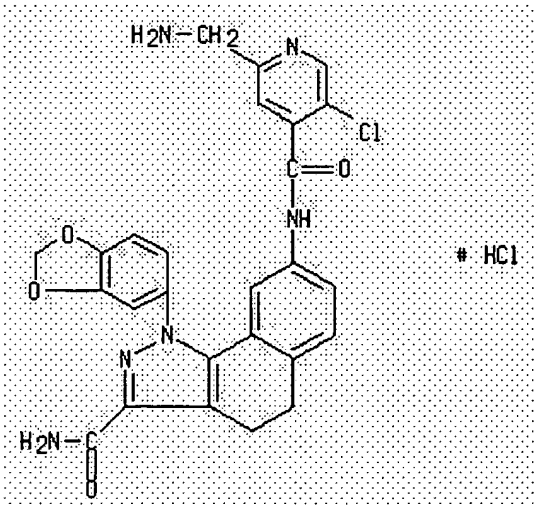
RN 623585-60-4 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[2-(aminomethyl)-5-chloro-4-pyridinyl]carbonyl]amino]-1-(4-fluorophenyl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)



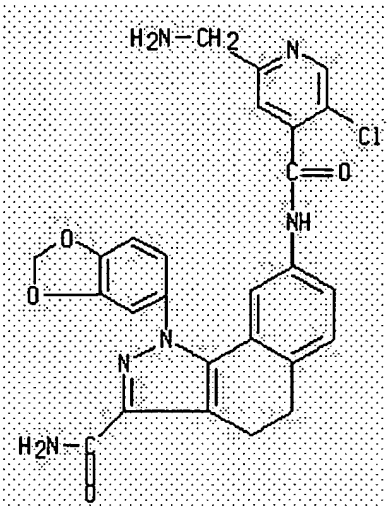
RN 623585-61-5 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[2-(aminomethyl)-5-chloro-4-pyridinyl]carbonyl]amino]-1-(4-fluorophenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 623585-63-7 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[2-(aminomethyl)-5-chloro-4-pyridinyl]carbonyl]amino]-1-(1,3-benzodioxol-5-yl)-4,5-dihydro-, monohydrochloride (9CI) (CA INDEX NAME)

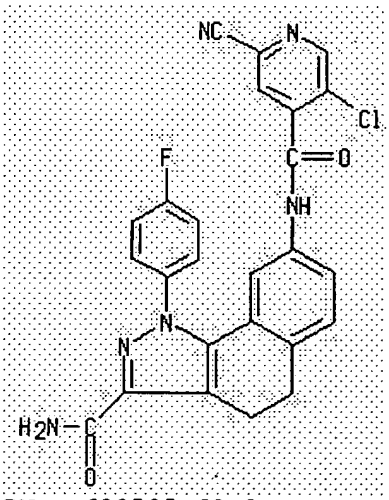


RN 623585-65-9 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[[2-(aminomethyl)-5-chloro-4-pyridinyl]carbonyl]amino]-1-(1,3-benzodioxol-5-yl)-4,5-dihydro- (9CI) (CA INDEX NAME)

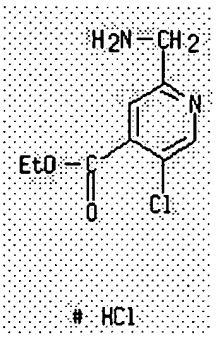


IT **623585-59-1P**, 8-[(5-Chloro-2-cyanoisonicotinoyl)amino]-1-(4-fluorophenyl)-4,5-dihydro-1H-benzo[g]indazole-3-carboxamide
623585-68-2P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 4,5-dihydro-1H-benzo[g]indazole-3-carboxamides as IKK2 inhibitors for treatment of cancer and inflammation)

RN 623585-59-1 HCAPLUS
CN 1H-Benz[g]indazole-3-carboxamide, 8-[[(5-chloro-2-cyano-4-pyridinyl)carbonyl]amino]-1-(4-fluorophenyl)-4,5-dihydro- (9CI) (CA INDEX NAME)



RN 623585-68-2 HCAPLUS
CN 4-Pyridinecarboxylic acid, 2-(aminomethyl)-5-chloro-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 13 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:875173 HCAPLUS
DOCUMENT NUMBER: 139:381511
TITLE: Pyrrolotriazine aniline compounds useful as kinase inhibitors, particularly p38 kinases, and their preparation, pharmaceutical compositions, and use as antiinflammatory agents
INVENTOR(S): Dyckman, Alaric; Hynes, John; Leftheris, Katherina; Liu, Chunjian; Wrobleski, Stephen T.
PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA
SOURCE: PCT Int. Appl., 158 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

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WO 2003090912	A1	20031106	WO 2003-US12426		20030415
WO 2003090912	C2	20040108			
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AU 2003231034	A1	20031110	AU 2003-231034		20030415
EP 1497019	A1	20050119	EP 2003-724157		20030415
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JP 2005523338	T2	20050804	JP 2003-587532		20030415
CN 1662509	A	20050831	CN 2003-814293		20030415
NO 2004004560	A	20041110	NO 2004-4560		20041022
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OTHER SOURCE(S): MARPAT 139:381511
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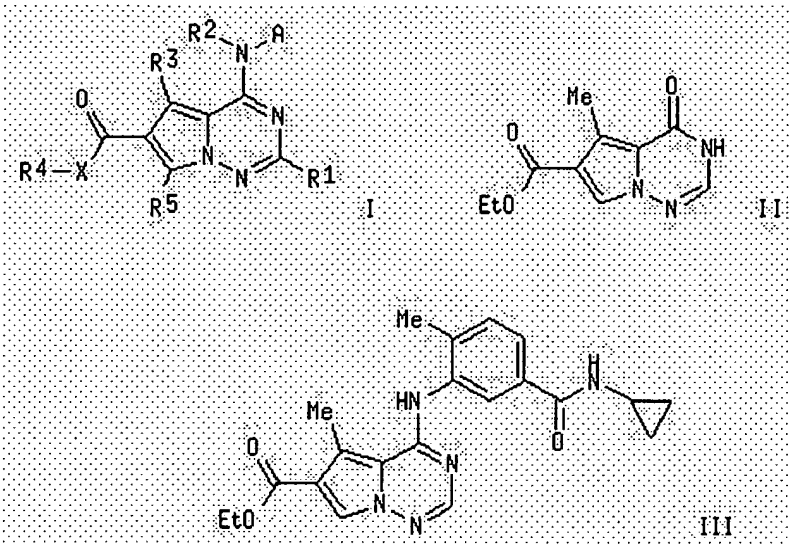
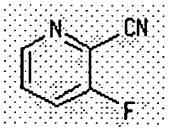


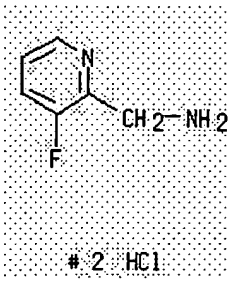
AB Title compds. I and their enantiomers, diastereomers, pharmaceutically acceptable salts, prodrugs, and solvates are useful as p38 kinase inhibitors [wherein: A = certain substituted Ph rings, particularly bearing various carboxamide and sulfonamide substituents; X = O, OCO, S, S(O), SO2, CO, CO2, (un)substituted NH, NHCO, NHCONH, NHCO2, NHSO2, NHSO2NH, SO2NH, or CONH, halo, NO2, cyano, or bond; R1, R5 = H, (un)substituted alkyl, OH or derivs., SH or derivs, CO2H or derivs., NH2 or derivs., halo, NO2, cyano; R2 = H, alkyl; R3 = H, Me, CF3, MeO, halo, cyano, NH2, or NHMe; R4 = H (with provisos), (un)substituted alk(en/yn)yl, (hetero)aryl, (hetero)cycloalkyl, or absent]. Over 300 specific compds. I and various intermediates were prepd. Compds. I selectively inhibited human p38α/β isoenzymes and TNF-α in vitro (no data).
For instance, 3-amino-4-methylbenzoic acid was amidated quant. with cyclopropylamine using EDC and DMAP in DMF. The pyrrolotriazinone ester II was then chlorinated at the ring oxo group with POCl3 (100%). Aminolysis of the resulting chloride with the benzamide product from the first step gave 80% invention compd. III.

IT **97509-75-6P 312904-49-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of pyrrolotriazine aniline compds. as p38 kinase inhibitors)

RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | CHIP Related Articles

ACCESSION NUMBER: 2003:855655 HCAPLUS
DOCUMENT NUMBER: 139:350636
TITLE: Preparation of amino heteroaryl amides for use in pharmaceutical compositions for the treatment of angiogenesis mediated diseases such as cancer
INVENTOR(S): Patel, Vinod F.; Askew, Benny; Booker, Shon; Chen, Guoqing; Dipietro, Lucian V.; Germain, Julie; Habgood, Gregory J.; Huang, Qi; Kim, Tae-seong; Li, Aiwen; Nishimura, Nobuko; Nomak, Rana; Riahi, Babak; Yuan, Chester Chenguang; Elbaum, Daniel
PATENT ASSIGNEE(S): Amgen Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 148 pp., Cont.-in-part of U.S. Ser. No. 46,622.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003203922	A1	20031030	US 2002-197918	20020717
US 2003195230	A1	20031016	US 2002-46622	20020110
CN 1538836	A	20041020	CN 2002-806467	20020111
ZA 2003005198	A	20040630	ZA 2003-5198	20030704
CA 2492045	AA	20040122	CA 2003-2492045	20030715
WO 2004007481	A2	20040122	WO 2003-US22275	20030715
WO 2004007481	A3	20040219		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003263784	A1	20040202	AU 2003-263784	20030715
EP 1562933	A2	20050817	EP 2003-764755	20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006502118	T2	20060119	JP 2004-521922	20030715
PRIORITY APPLN. INFO.:			US 2001-261882P	P 20010112
			US 2001-323808P	P 20010919

US 2002-46622 A2 20020110
US 2002-197918 A 20020717
WO 2003-US22275 W 20030715

OTHER SOURCE(S): MARPAT 139:350636

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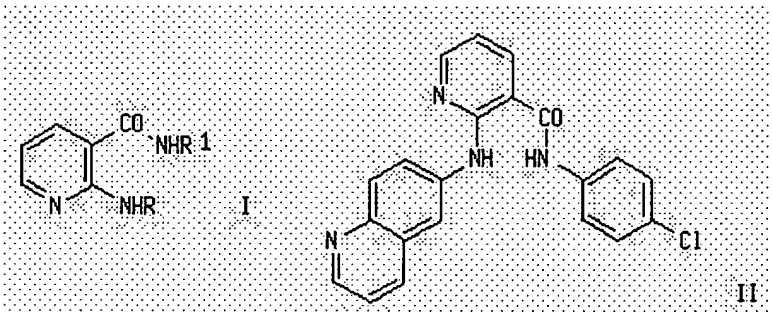
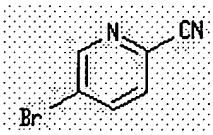


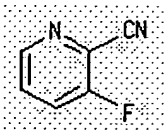
AB Amino substituted heteroaryl amides, such as I [R = nitrogen contg. heteroaryl, such as quinolinyl, isoquinolinyl, indazolyl; R1 = aryl, cycloalkyl, heteroaryl, heterocyclyl], were prepd. for therapeutic use. The invention encompasses novel compds., analogs, prodrugs and pharmaceutically acceptable salts thereof, pharmaceutical compns. and methods for prophylaxis and treatment of cancer, angiogenesis related disorders, KDR-related disorders, cell proliferation related disorders, inflammation, reducing blood flow in tumors, reducing tumor size and diabetic retinopathy. Thus, amide II was prepd. via an amination reaction of 2-chloronicotinic acid with 6-aminoquinoline followed by an amidation reaction of the aminonicotinic acid deriv. thus formed with 4-chloroaniline. Biol. evaluations included HUVEC proliferation assay, inhibition of angiogenesis in the rat corneal neovascularization micropocket model, and antitumor activity using A431 rat tumor cells.

IT **97483-77-7P**, 5-Bromopyridine-2-carbonitrile **97509-75-6P**
312904-51-1P **327056-62-2P** **561297-96-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of aminopyridinecarboxamides for therapeutic use in treatment of angiogenesis mediated diseases such as cancer)

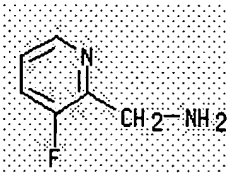
RN 97483-77-7 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-bromo- (9CI) (CA INDEX NAME)



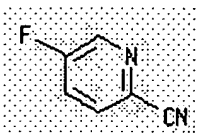
RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



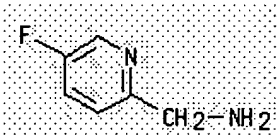
RN 312904-51-1 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro- (9CI) (CA INDEX NAME)



RN 327056-62-2 HCAPLUS
CN 2-Pyridinecarbonitrile, 5-fluoro- (9CI) (CA INDEX NAME)



RN 561297-96-9 HCAPLUS
CN 2-Pyridinemethanamine, 5-fluoro- (9CI) (CA INDEX NAME)



L11 ANSWER 15 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:551181 HCAPLUS
DOCUMENT NUMBER: 139:117339
TITLE: Preparation of substituted arylamine derivatives as antitumor agents
INVENTOR(S): Elbaum, Daniel; Askew, Benny; Booker, Shon; Germain, Julie; Habgood, Gregory; Handley, Michael; Kim, Tae-Seong; Li, Aiwen; Nishimura, Nobuko; Patel, Vinod F.; Yuan, Chester Chenguang; Kim, Joseph L.
PATENT ASSIGNEE(S): Amgen Inc., USA
SOURCE: U.S. Pat. Appl. Publ., 106 pp., Cont.-in-part of U.S. Ser. No. 46,526.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003134836	A1	20030717	US 2002-197960	20020717
US 2002147198	A1	20021010	US 2002-46526	20020110
CA 2492164	AA	20040122	CA 2003-2492164	20030715
WO 2004007457	A2	20040122	WO 2003-US22276	20030715
WO 2004007457	A3	20050804		

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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2003256577	A1	20040202	AU 2003-256577	20030715
EP 1583744	A2	20051012	EP 2003-764756	20030715
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2006505511	T2	20060216	JP 2004-521923	20030715
US 2004204437	A1	20041014	US 2004-823809	20040412
US 2005153960	A1	20050714	US 2004-996035	20041122
PRIORITY APPLN. INFO.:			US 2001-261360P	P 20010112
			US 2001-323686P	P 20010919
			US 2002-46526	A2 20020110
			US 2002-197960	A 20020717
			WO 2003-US22276	W 20030715
			US 2004-823809	A1 20040412

OTHER SOURCE(S): MARPAT 139:117339

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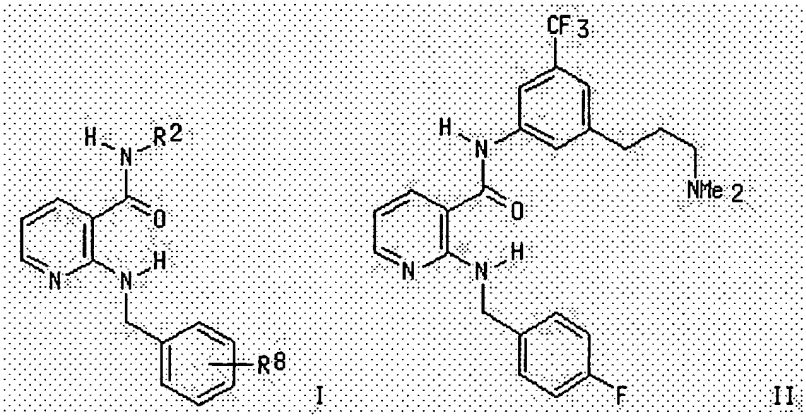
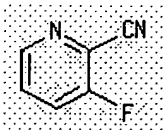


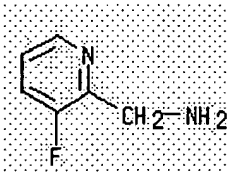
AB The title compds. I [R2 = (un)substituted Ph, 9-10 membered bicyclic and 11-14 membered tricyclic (un)satd. heterocyclyl; R8 = halo, NH2, NO2, etc.], and their pharmaceutically acceptable derivs., are prepd. and disclosed as agents effective for prophylaxis and treatment of diseases, such as angiogenesis mediated diseases. E.g., a multi-step synthesis of II, starting from 1-dimethylamino-2-propyne and 3-bromo-5-trifluoromethylaniline, was given. Selected compds. of the invention, e.g., II, inhibited VEGF-stimulated cell proliferation at a level below 50 nM. The invention encompasses novel compds., analogs, prodrugs and pharmaceutically acceptable derivs. thereof, pharmaceutical compns. and methods for prophylaxis and treatment of diseases and other maladies or conditions involving, cancer and the like.

IT **97509-75-6P 312904-51-1P 561297-96-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of substituted aminopyridines as antitumor agents)

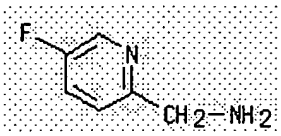
RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



RN 312904-51-1 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro- (9CI) (CA INDEX NAME)



RN 561297-96-9 HCAPLUS
CN 2-Pyridinemethanamine, 5-fluoro- (9CI) (CA INDEX NAME)



L11 ANSWER 16 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:490976 HCAPLUS
DOCUMENT NUMBER: 139:69151
TITLE: Preparation of pyridinecarboxamides and -sulfonamides as bradykinin B2 receptor antagonists
INVENTOR(S): Cheng, Yun-Xing; Luo, Xuehong; Tomaszewski, Miroslaw; Walpole, Christopher
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 191 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003051276	A2	20030626	WO 2002-SE2354	20021217
WO 2003051276	A3	20031120		
WO 2003051276	B1	20040408		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2468978	AA	20030626	CA 2002-2468978	20021217
AU 2002359150	A1	20030630	AU 2002-359150	20021217
EP 1458684	A2	20040922	EP 2002-793663	20021217
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2005518374	T2	20050623	JP 2003-552210	20021217
US 2005245503	A1	20051103	US 2004-498864	20040616
PRIORITY APPLN. INFO.:			SE 2001-4326 A	20011219
			WO 2002-SE2354 W	20021217

OTHER SOURCE(S): MARPAT 139:69151
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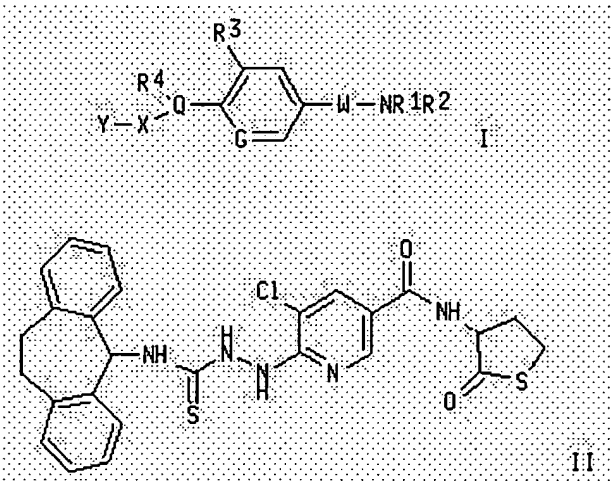
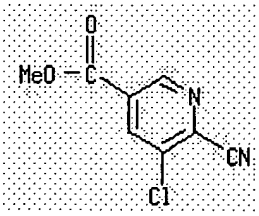


AB Pyridines I [G, Q = N, CH; W = linking group; X = (un)substituted NHCH2NH, NHCH:CHNH; Y = dibenzocycloheptyl, heterodibenzocycloheptyl; R1, R2 = H, acyl, alkoxycarbonyl, (un)substituted alkyl, cycloalkyl, aryl, heterocyclyl; R3 = H, halogen, alkyl; R4 = h, (un)substituted hydrocarbyl] were prepd. for use as bradykinin B2 receptor antagonists in the treatment of pain and have Ki for human B2 receptor binding of 5-5000 nM. Thus, 5-amino-10,11-dihydrodibenzo[a,d]cycloheptene was converted to the isothiocyanate and treated with 5-chloro-6-hydrazinonicotinic acid, followed by D-homocysteine thiolactone to give the pyridinecarboxamide II.

IT **398457-04-0P** **549531-03-5P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of pyridinecarboxamides and -sulfonamides as bradykinin B2 receptor antagonists)

RN 398457-04-0 HCAPLUS
CN 3-Pyridinecarboxylic acid, 5-chloro-6-cyano-, methyl ester (9CI) (CA INDEX NAME)



RN 549531-03-5 HCAPLUS
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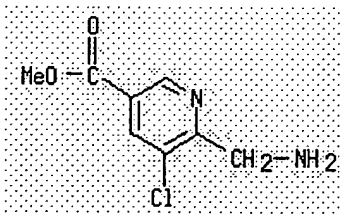

L11 ANSWER 17 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2003:454299 HCAPLUS
DOCUMENT NUMBER: 139:36535
TITLE: Preparation of pyrimidine derivatives as modulators of insulin-like growth factor-1 receptor (IGF-1)
INVENTOR(S): Barlaam, Bernard; Pape, Andrew; Thomas, Andrew
PATENT ASSIGNEE(S): Astrazeneca AB, Swed.
SOURCE: PCT Int. Appl., 78 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2003048133	A1	20030612	WO 2002-SE2221		20021203
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG					
CA 2467838	AA	20030612	CA 2002-2467838		20021203
AU 2002365864	A1	20030617	AU 2002-365864		20021203
BR 2002014605	A	20040914	BR 2002-14605		20021203
EP 1456182	A1	20040915	EP 2002-791165		20021203
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK					
CN 1617858	A	20050518	CN 2002-827802		20021203
JP 2005515998	T2	20050602	JP 2003-549325		20021203
ZA 2004004223	A	20050829	ZA 2004-4223		20040528
NO 2004002872	A	20040706	NO 2004-2872		20040706
US 2005054638	A1	20050310	US 2004-497744		20041108
PRIORITY APPLN. INFO.:			SE 2001-4140	A	20011207
			WO 2002-SE2221	W	20021203

OTHER SOURCE(S): MARPAT 139:36535
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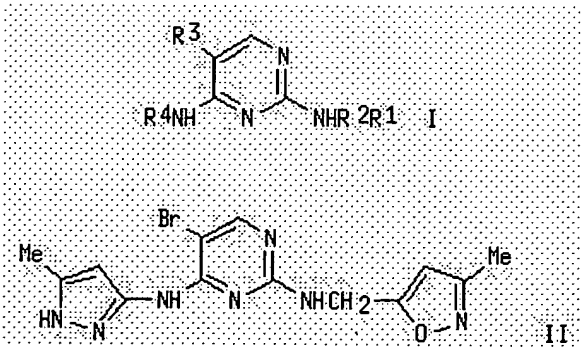
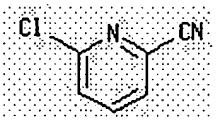


AB Pyrimidinediamines I [R1, R4 = (un)substituted heteroarom.; R2 = alkyl, haloalkyl, hydroxyalkyl, alkoxy (sic); R3 = H, halogen, CF3] were prepd. for use as modulators of IGF-1 in the treatment of cancer with IC50 in the IGF-1R kinase assay of ? 100 μM and in the IGF-stimulated cell proliferation test of ? 50 μM. Thus, 5-bromo-2,4-dichloropyrimidine was treated with 3-amino-5-methyl-1H-pyrazole, followed by 5-aminomethyl-3-methylisoxazole hydrochloride to give the diamine II.

IT **33252-29-8**, 6-Chloro-2-pyridinecarbonitrile
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of pyrimidine derivs. as modulators of insulin-like growth factor-1 receptor (IGF-1))

RN 33252-29-8 HCAPLUS

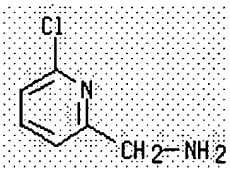
CN 2-Pyridinecarbonitrile, 6-chloro- (9CI) (CA INDEX NAME)



IT **188637-75-4P**, 2-Aminomethyl-6-chloropyridine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of pyrimidine derivs. as modulators of insulin-like growth factor-1 receptor (IGF-1))

RN 188637-75-4 HCAPLUS

CN 2-Pyridinemethanamine, 6-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 18 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Cited References

ACCESSION NUMBER: 2003:16682 HCAPLUS

DOCUMENT NUMBER: 138:198146

TITLE: Metabolism-Directed Optimization of 3-Aminopyrazinone Acetamide Thrombin Inhibitors. Development of an Orally Bioavailable Series Containing P1 and P3 Pyridines

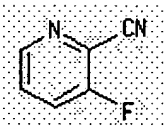
AUTHOR(S): Burgey, Christopher S.; Robinson, Kyle A.; Lyle, Terry A.; Sanderson, Philip E. J.; Lewis, S. Dale; Lucas, Bobby J.; Krueger, Julie A.; Singh, Rominder; Miller-Stein, Cynthia; White, Rebecca B.; Wong, Bradley; Lyle, Elizabeth A.; Williams, Peter D.; Coburn, Craig A.; Dorsey, Bruce D.; Barrow, James C.; Stranieri, Maria T.; Holahan, Marie A.; Sitko, Gary R.; Cook, Jacquelynn J.; McMasters, Daniel R.; McDonough, Colleen M.; Sanders, William M.; Wallace, Audrey A.; Clayton, Franklin C.; Bohn, Dennis; Leonard, Yvonne M.; Detwiler, Theodore J., Jr.; Lynch, Joseph J., Jr.; Yan, Youwei; Chen, Zhongguo; Kuo, Lawrence; Gardell, Stephen J.; Shafer, Jules A.; Vacca, Joseph P.

CORPORATE SOURCE: Departments of Medicinal Chemistry, Biological Chemistry, Drug Metabolism Molecular Systems, Structural Biology and Pharmacology, Merck Research Laboratories, West Point, PA, 19486, USA
SOURCE: Journal of Medicinal Chemistry (2003), 46(4), 461-473
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:198146

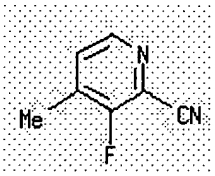
AB Recent efforts in the field of thrombin inhibitor research have focused on the identification of compds. with good oral bioavailability and pharmacokinetics. In this manuscript we describe a metab.-based approach to the optimization of the 3-(2-phenethylamino)-6-methylpyrazinone acetamide template which resulted in the modification of each of the three principal components (i.e., P1, P2, P3) comprising this series. As a result of these studies, several potent thrombin inhibitors were identified which exhibit high levels of oral bioavailability and long plasma half-lives.

IT **97509-75-6** **312904-99-7**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(metab.-directed optimization of 3-aminopyrazinone acetamide thrombin inhibitors and structure-activity relationship)

RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



RN 312904-99-7 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro-4-methyl- (9CI) (CA INDEX NAME)



IT **38180-46-0P** **312905-00-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(metab.-directed optimization of 3-aminopyrazinone acetamide thrombin inhibitors and structure-activity relationship)

RN 38180-46-0 HCAPLUS
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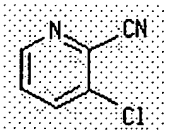
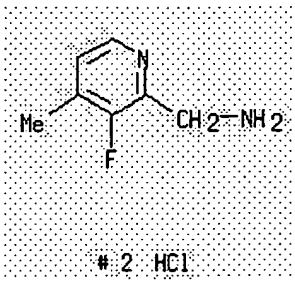
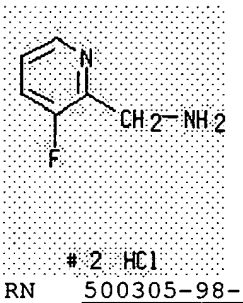


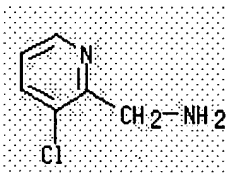
RN 312905-00-3 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



IT 312904-49-7P 500305-98-6P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(metab.-directed optimization of 3-aminopyrazinone acetamide thrombin inhibitors and structure-activity relationship)
RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



RN 500305-98-6 HCAPLUS
CN 2-Pyridinemethanamine, 3-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

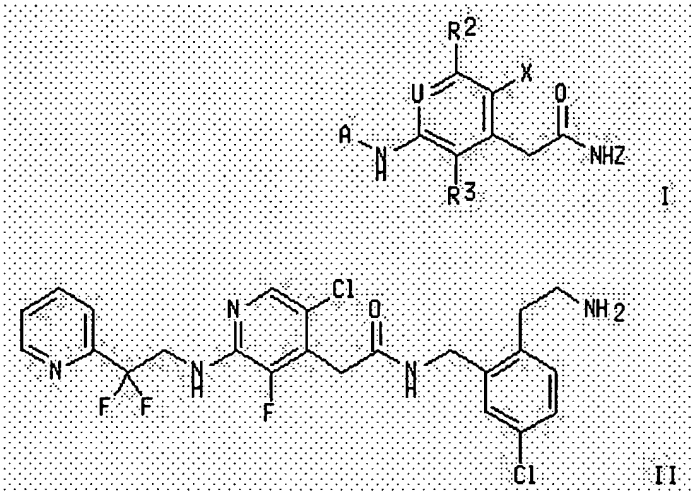
L11 ANSWER 19 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Charg References

ACCESSION NUMBER: 2002:965130 HCAPLUS
DOCUMENT NUMBER: 138:39286
TITLE: Preparation of 2-(pyridin-4-yl)acetamides as thrombin inhibitors
INVENTOR(S): Barrow, James C.; Coburn, Craig; Selnick, Harold G.; Ngo, Phung L.
PATENT ASSIGNEE(S): USA
SOURCE: U.S. Pat. Appl. Publ., 61 pp.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

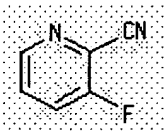
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002193398	A1	20021219	US 2002-71422	20020208
US 6610701	B2	20030826		
PRIORITY APPLN. INFO.:			US 2001-267960P P	20010209

OTHER SOURCE(S): MARPAT 138:39286
GI

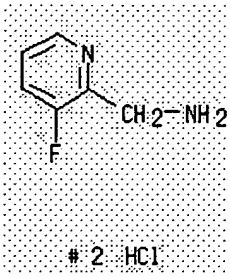


AB The title compds. [I; U = N, CH; A = CH2CY2R1, SO2CH2R1; R1 = (un)substituted unsatd. 6-membered non-heterocyclyl, satd. 6-membered heterocyclyl, 1-oxidopyridyl; R2 = H, F; R3 = H, halo; X = H, halo, alkyl, CN, CF3; Y = H, alkyl, F; Z = CR12R13(CH2)0-1R4; R4 = (un)substituted unsatd. 6-membered non-heterocyclyl, unsatd. 6-membered monocyclic heterocyclyl, unsatd. 9-10 membered bicyclic heterocyclyl, CH2CONHC(:NH)NH2; R12, R13 = H, alkyl] and their salts, useful in inhibiting thrombin and treating blood coagulation and cardiovascular disorders, were prepd. and formulated. E.g., a multi-step synthesis of II which showed Ki of < 20 nM against human thrombin, was given.

IT **97509-75-6**, 2-Cyano-3-fluoropyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of 2-(pyridin-4-yl)acetamides as thrombin inhibitors)
RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



IT **312904-49-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 2-(pyridin-4-yl)acetamides as thrombin inhibitors)
RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



L11 ANSWER 20 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

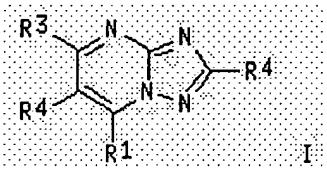
Full Text | Citing References

ACCESSION NUMBER: 2002:637565 HCAPLUS
DOCUMENT NUMBER: 137:185499
TITLE: Preparation of triazolopyrimidines as thrombin inhibitors
INVENTOR(S): Williams, Peter D.; Coburn, Craig; Burgey, Christopher; Morrissette, Matthew M.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 184 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002064211	A1	20020822	WO 2002-US4654	20020205

W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

PRIORITY APPLN. INFO.: US 2001-267813P P 20010209
OTHER SOURCE(S): MARPAT 137:185499
GI

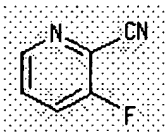


I

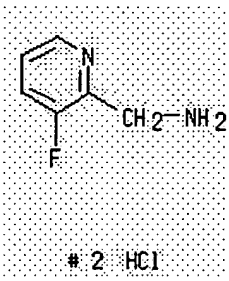
AB Title compds. [I; R1 = H, halo, OH, NH(CH2)nR5, NHCH2CF2R5, etc.; n = 1-3; R2 = H, (CH2)mR6, SO2R6; m = 0-2; R3 = H, alkyl, cycloalkyl, CF3; R2R3 = atoms to form a 5-7 membered nonheterocyclic ring; R4 = CH2R7, NH(CH2)mR7; R5 = H, pyridine oxide, tetrahydrothiophene dioxide, (substituted) (hetero)cyclyl, etc.; R6 = pyridine oxide, (substituted) (hetero)cyclyl, etc.; R7 = (substituted) Ph, pyridyl], were prepd. Thus, 3-(2-methyl-5-chlorophenylamino)-5-amino-1,2,4-triazole (prepn. given) and Et acetoacetate in HOAc were heated to reflux for 18 h. to give 2-(2-methyl-5-chlorophenylamino)-5-methyl-7-hydroxy-1,2,4-triazolo[1,5-a]pyrimidine. The latter was refluxed 1 h with POCl3 to give the 7-chloro deriv. which was heated with 2-(2-pyridyl)ethylamine at 100? for 30 min. to give 2-(2-methyl-5-chlorophenylamino)-5-methyl-7-[2-(2-pyridyl)ethylamino]-1,2,4-triazolo[1,5-a]pyrimidine dihydrochloride (II). I inhibited thrombin with IC50<24 nM. II drug compns. are given.

IT **97509-75-6**, 3-Fluoro-2-pyridinenitrile
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of triazolopyrimidines as thrombin inhibitors)

RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



IT **312904-49-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of triazolopyrimidines as thrombin inhibitors)
RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 21 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | String References

ACCESSION NUMBER: 2002:157737 HCAPLUS
DOCUMENT NUMBER: 136:200109
TITLE: Process for preparation of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines.
INVENTOR(S): Dann, Norman; Riordan, Peter Dominic; Amin, Mehul Rasikchandra; Mellor, Michael
PATENT ASSIGNEE(S): Aventis CropScience SA, Fr.
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002016322	A2	20020228	WO 2001-EP10984	20010821
WO 2002016322	A3	20020606		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1199305	A1	20020424	EP 2001-420128	20010607
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
CA 2415842	AA	20020228	CA 2001-2415842	20010821

AU 2002013948	A5	20020304	AU 2002-13948	20010821
EP 1311483	A2	20030521	EP 2001-982337	20010821
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2001013259	A	20030715	BR 2001-13259	20010821
JP 2004506716	T2	20040304	JP 2002-521198	20010821
RU 2266900	C2	20051227	RU 2003-107931	20010821
CN 1721406	A	20060118	CN 2005-10088220	20010821
US 2004049048	A1	20040311	US 2003-362728	20030611
US 6921828	B2	20050726		
US 2005250947	A1	20051110	US 2005-177118	20050708
PRIORITY APPLN. INFO.:			GB 2000-21066 A	20000825
			GB 2000-25616 A	20001019
			EP 2001-420128 A	20010607
			CN 2001-814622 A3	20010821
			WO 2001-EP10984 W	20010821
			US 2003-362728 A1	20030611

OTHER SOURCE(S): CASREACT 136:200109; MARPAT 136:200109

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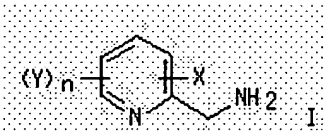
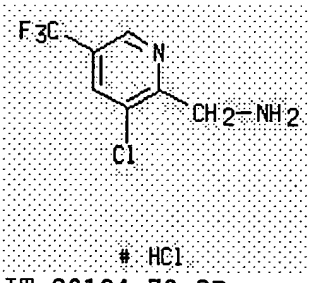


AB Title compds. (I; X = halo; Y = halo, haloalkyl, alkoxycarbonyl, alkylsulfonyl; n = 0-3) were prepd. by catalytic hydrogenation of the corresponding 2-cyano derivs. Thus, 3-chloro-2-cyano-5-trifluoromethylpyridine (prepn. given) was hydrogenated in MeOH over Pd/C contg. HCl at 1 atm. to give 95-97% 2-aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride.

IT **326476-49-7P**, 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(process for prepn. of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines)

RN 326476-49-7 HCAPLUS

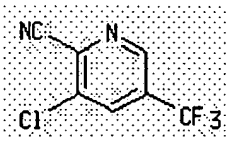
CN 2-Pyridinemethanamine, 3-chloro-5-(trifluoromethyl)-, monohydrochloride (9CI) (CA INDEX NAME)



IT **80194-70-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process for prepn. of 2-aminomethylpyridines by catalytic hydrogenation of 2-cyanopyridines)

RN 80194-70-3 HCAPLUS

CN 2-Pyridinecarbonitrile, 3-chloro-5-(trifluoromethyl)- (9CI) (CA INDEX NAME)



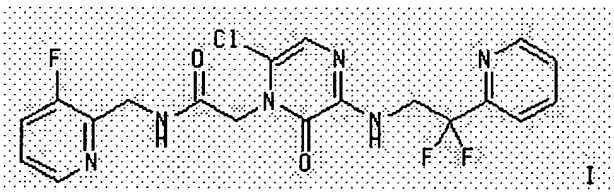
L11 ANSWER 22 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:886079 HCAPLUS
DOCUMENT NUMBER: 136:6012
TITLE: Pyrazinone thrombin inhibitors, namely N-((3-fluoro-2-pyridyl)methyl)-3-((2,2-difluoro-2-(2-pyridyl)ethyl)amino)-6-chloropyrazin-2-one-1-acetamide anhydrous and monohydrate polymorphs, and their preparation and use as antithrombotics
INVENTOR(S): Cowden, Cameron J.; Cooper, V. Brett; Rush, Daniel J.; Frech, Patricia
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 31 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001092234	A1	20011206	WO 2001-US17268	20010525
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002004507	A1	20020110	US 2001-870560	20010531
US 6521625	B2	20030218		

PRIORITY APPLN. INFO.: US 2000-208665P P 20000601
GI



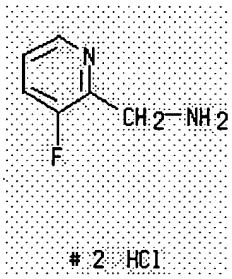
I

AB The compds. of the invention are cryst. polymorphs of N-((3-fluoro-2-pyridyl)methyl)-3-((2,2-difluoro-2-(2-pyridyl)ethyl)amino)-6-chloropyrazin-2-one-1-acetamide (I) and its monohydrate, useful in inhibiting thrombin (no data) and assocd. thrombotic occlusions. In particular, the invention compds. are selected from: I polymorphic cryst. anhyd. form B (IB), I polymorphic cryst.type A monohydrate (IA.H2O), and I polymorphic cryst. type B monohydrate (IB.H2O), or a pharmaceutically acceptable salt thereof. I was prepd. in 9 steps: (1) hydrogenation of

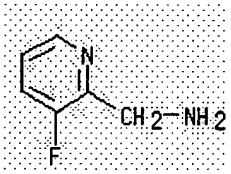
2-cyano-3-fluoropyridine to give 2-aminomethyl-3-fluoropyridine di-HCl (II); (2) condensation of H2NCH2CO2Et with ClCOCO2Et to give EtO2CCONHCH2CO2Et; (3) amidation of the latter with (MeO)2CHCH2NH2; (4) acid cyclization of the product to give Et 3-hydroxypyrazin-2(1H)-one-1-acetate; (5) treatment of the latter with POBr3 to give Et 3-bromopyrazin-2(1H)-one-1-acetate; (6) coupling of this bromide with 2,2-difluoro-2-(2-pyridyl)ethylamine; (7) chlorination of the 6-position with NCS; (8) alk. sapon. of the ester, and (9) amidation of the acid with II. The polymorphs were obtained by crystn. from the following solvents: IA from 2-methyl-1-propanol, m.p. 185?; IB from 2-butanone, m.p. 179?; IA.H2O from aq. MeCN; and IB.H2O from aq. 2-propanol contg. aq. HCl. The 4 forms gave characteristic X-ray powder diffractograms. Several pharmaceutical forms are also described.

IT **312904-49-7P**, 2-(Aminomethyl)-3-fluoropyridine dihydrochloride
312904-51-1P, 2-(Aminomethyl)-3-fluoropyridine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(intermediate; prepn. of pyrazinone deriv. polymorphs as thrombin inhibitors)

RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)

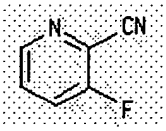


RN 312904-51-1 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro- (9CI) (CA INDEX NAME)



IT **97509-75-6**, 2-Cyano-3-fluoropyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(precursor; prepn. of pyrazinone deriv. polymorphs as thrombin inhibitors)

RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

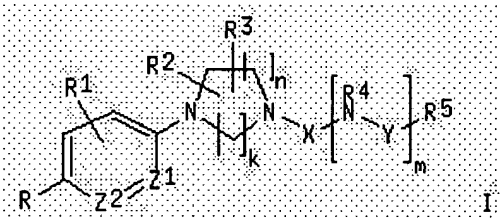
L11 ANSWER 23 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:857479 HCAPLUS
DOCUMENT NUMBER: 136:600
TITLE: Pharmaceuticals containing antiandrogen cyanophenyl compounds
INVENTOR(S): Taniguchi, Nobuaki; Kinoyama, Isao; Kamikubo, Takashi; Toshima, Hiroshi; Samizu, Kiyohiro; Kawanami, Eiji; Imamura, Masakazu; Moritomo, Hiroyuki; Matsuhisa, Akira; Hirano, Hiroaki; Miyasaki, Yoji; Nozawa, Shigenori; Okada, Minoru; Koutoku, Hiroshi; Ota, Mitsuaki
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 33 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001328938	A2	20011127	JP 2001-69833	20010313
PRIORITY APPLN. INFO.:			JP 2000-75008 A	20000317

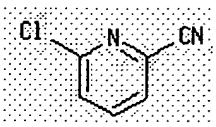
OTHER SOURCE(S): MARPAT 136:600
GI



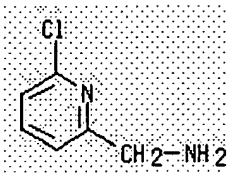
I

AB Pharmaceuticals, useful for treatment of prostatic cancer, prostatic hypertrophy, virilism, etc., contain cyanophenyl compds. I [R = cyano, NO2; R1 = H, halo, cyano, haloalkyl, NO2, etc.; R2-R4 = H, lower alkyl, (alkyl)carbamoyl, etc.; R5 = lower alkyl, arylalkoxy, CO2H, lower alkoxycarbonyl, etc.; X = CO, C(S), SO2; Y = bond, lower alkylene, CO, SO2; Z1, Z2 = CH, N; k, n = 1-3; m = 0, 1] or their salts. (2R,5S)-I (R = cyano, R1 = 3-CF3, R2 = 2-Me, R3 = 5-Me, k = 2, m = n = 1, X = CO, R4 = H, R5 = 2-bromo-4-pyridyl) (prepn. given) in vitro bound to rat androgen receptor with Ki of 7.56 nM.

IT **33252-29-8**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of cyanophenyl compds. as antiandrogens)
RN 33252-29-8 HCAPLUS
CN 2-Pyridinecarbonitrile, 6-chloro- (9CI) (CA INDEX NAME)



IT **188637-75-4P**, 2-Aminomethyl-6-chloropyridine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of cyanophenyl compds. as antiandrogens)
RN 188637-75-4 HCAPLUS
CN 2-Pyridinemethanamine, 6-chloro- (9CI) (CA INDEX NAME)



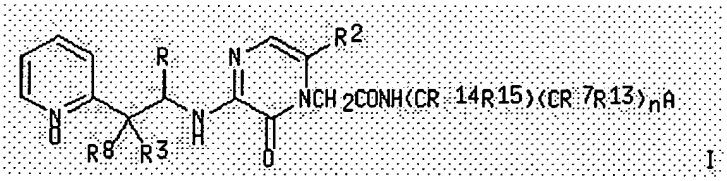
L11 ANSWER 24 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2001:396862 HCAPLUS
DOCUMENT NUMBER: 135:19662
TITLE: Preparation of pyrazinones as thrombin inhibitors.
INVENTOR(S): Burgey, Christopher; Isaacs, Richard C.; Dorsey, Bruce D.; Robinson, Kyle A.; Staas, Donnette; Sanderson, Philip E.; Barrow, James
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 137 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2001038323	A1	20010531	WO 2000-US31787		20001120
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2391012	AA	20010531	CA 2000-2391012		20001120
EP 1259506	A1	20021127	EP 2000-983727		20001120
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR					
JP 2003514905	T2	20030422	JP 2001-540086		20001120
US 6387911	B1	20020514	US 2000-717566		20001121
PRIORITY APPLN. INFO.:			US 1999-167070P	P	19991123
			US 2000-216889P	P	20000707
			WO 2000-US31787	W	20001120

OTHER SOURCE(S): MARPAT 135:19662
GI



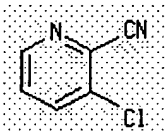
I

AB Title compds. [I; A = (substituted) pyridinyl (oxide), Ph; R = H, alkyl, haloalkyl, OR9, N(R9)2, CO2R9, etc.; R2 = H, alkyl, CF3, halo, cyano, cyanoalkyl; R3, R7, R8, R13 = H, halo, alkyl; R14, R15 = H, (substituted) alkyl; n = 0, 1], were prepd. (no data). Thus, 3-[2,2-difluoro-2-(2-

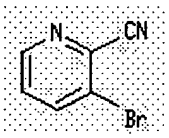
pyridyl-N-oxide)ethylamino]-6-chloropyrazin(1H)-2-one-1-acetic acid (prepn. given), 2-aminomethyl-3-fluoropyridine dihydrochloride, EDC, HOAT, and N-methylmorpholine were stirred overnight to give 3-fluoro-2-pyridylmethyl-3-[2,2-difluoro-2-(2-pyridyl-N-oxide)ethylamino]-6-chloropyrazin-2-one-1-acetamide. Drug formulations contg. the latter were given.

IT **38180-46-0**, 3-Chloro-2-cyanopyridine **55758-02-6**, 3-Bromo-2-cyanopyridine **97509-75-6**, 2-Cyano-3-fluoropyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of pyrazinones as thrombin inhibitors)

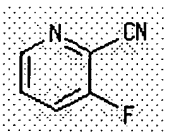
RN 38180-46-0 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-chloro- (9CI) (CA INDEX NAME)



RN 55758-02-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-bromo- (9CI) (CA INDEX NAME)

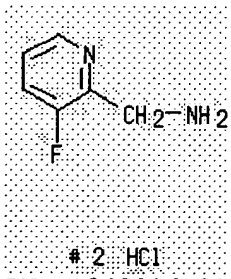


RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)

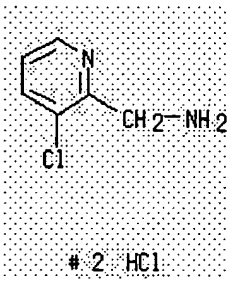


IT **312904-49-7P** **342816-31-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of pyrazinones as thrombin inhibitors)

RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



RN 342816-31-3 HCAPLUS
CN 2-Pyridinemethanamine, 3-chloro-, dihydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 25 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | CAPLUS References

ACCESSION NUMBER: 2000:881144 HCAPLUS
DOCUMENT NUMBER: 134:42142
TITLE: Preparation of pyrazinone thrombin inhibitors
INVENTOR(S): Burgey, Christopher S.; Robinson, Kyle A.; Williams, Peter D.; Coburn, Craig A.; Lyle, Terry A.; Sanderson, Philip E.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: PCT Int. Appl., 98 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000075134	A1	20001214	WO 2000-US15140	20000601
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2373999	AA	20001214	CA 2000-2373999	20000601
BR 2000011260	A	20020319	BR 2000-11260	20000601
EP 1189899	A1	20020327	EP 2000-939492	20000601
EP 1189899	B1	20030212		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6455532	B1	20020924	US 2000-585112	20000601
TR 200103491	T2	20021223	TR 2001-200103491	20000601
JP 2003501426	T2	20030114	JP 2001-502417	20000601
AT 232527	E	20030215	AT 2000-939492	20000601
EE 200100641	A	20030217	EE 2001-641	20000601
AU 761982	B2	20030612	AU 2000-54571	20000601
ES 2190417	T3	20030801	ES 2000-939492	20000601
NZ 515454	A	20040227	NZ 2000-515454	20000601
ZA 2001009774	A	20021128	ZA 2001-9774	20011128
NO 2001005887	A	20020123	NO 2001-5887	20011203
HR 2001000903	A1	20030430	HR 2001-903	20011204
BG 106263	A	20020628	BG 2001-106263	20011221

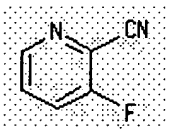
PRIORITY APPLN. INFO.: US 1999-137538P P 19990604
US 1999-144291P P 19990716
WO 2000-US15140 W 20000601

OTHER SOURCE(S): MARPAT 134:42142
GI

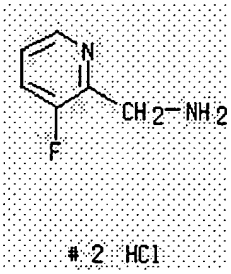
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB The title compds. [I; W = H, (un)satd. (un)substituted 5-7 membered mono- or 9-10 membered fused bicyclic heterocyclic ring, (un)substituted 5-7 membered or 9-10 membered fused bicyclic nonheterocyclic satd. ring, etc.; R3, X = H, halo, CN, etc.; A = II-IV (wherein Y1, Y2 = H, alkyl, alkoxy, etc.; b = 0-1)], useful in inhibiting thrombin and assocd. thrombotic occlusions, were prepd. and formulated. E.g., a multi-step synthesis of V which showed Ki of ? 1 nM in vitro assay of human α-thrombin, was given.

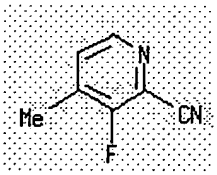
IT **97509-75-6**, 2-Cyano-3-fluoropyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of pyrazinone thrombin inhibitors)
RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



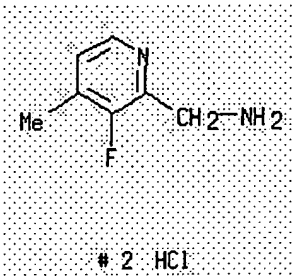
IT **312904-49-7P 312904-99-7P 312905-00-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of pyrazinone thrombin inhibitors)
RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



RN 312904-99-7 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro-4-methyl- (9CI) (CA INDEX NAME)



RN 312905-00-3 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-4-methyl-, dihydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 26 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 2000:880965 HCAPLUS
DOCUMENT NUMBER: 134:42134
TITLE: Preparation of 1,2,4,8-tetrahydro-2,8-dioxo-7H-pyrido[3,4-d][1,3]oxazine-7-acetamides as thrombin inhibitors
INVENTOR(S): Coburn, Craig A.; Burgey, Christopher S.
PATENT ASSIGNEE(S): Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 43 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
WO 2000074682	A1	20001214	WO 2000-US14921		20000531
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM					
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG					
CA 2374654	AA	20001214	CA 2000-2374654		20000531
EP 1189618	A1	20020327	EP 2000-939426		20000531
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO					
JP 2003501389	T2	20030114	JP 2001-501218		20000531
US 6350745	B1	20020226	US 2000-585740		20000602
PRIORITY APPLN. INFO.:			US 1999-137644P	P	19990604
			WO 2000-US14921	W	20000531

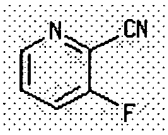
OTHER SOURCE(S): MARPAT 134:42134
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

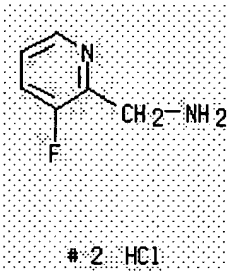
AB The title compds. [I; A = II-IV (wherein Y1, Y2 = H, alkyl, alkoxy, etc.;

b = 0-1); R1, R2 = H, (un)substituted Ph, CF3, etc.; R9 = alkyl] and their pharmaceutically acceptable salts, useful as thrombin inhibitors and having therapeutic value in for example, preventing coronary artery disease, were prepd. and formulated. Thus, reacting the carboxylic acid V with 3-fluoro-2-aminomethylpyridine in the presence of EDC, HOBT and N-methylmorpholine in DMF afforded VI.HCl which showed Ki of < 100 nM against human trypsin.

IT **97509-75-6**, 2-Cyano-3-fluoropyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of 1,2,4,8-tetrahydro-2,8-dioxo-7H-pyrido[3,4-d][1,3]oxazine-7-acetamides as thrombin inhibitors)
RN 97509-75-6 HCAPLUS
CN 2-Pyridinecarbonitrile, 3-fluoro- (9CI) (CA INDEX NAME)



IT **312904-49-7P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 1,2,4,8-tetrahydro-2,8-dioxo-7H-pyrido[3,4-d][1,3]oxazine-7-acetamides as thrombin inhibitors)
RN 312904-49-7 HCAPLUS
CN 2-Pyridinemethanamine, 3-fluoro-, dihydrochloride (9CI) (CA INDEX NAME)



REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 27 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Cited References

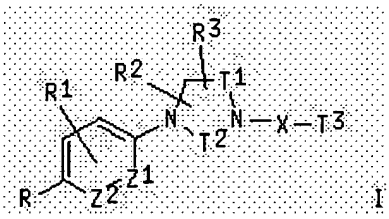
ACCESSION NUMBER: 2000:210118 HCAPLUS
DOCUMENT NUMBER: 132:237107
TITLE: Preparation of piperazino-substituted cyanophenyl derivatives as antiandrogen agents
INVENTOR(S): Taniguchi, Nobuaki; Kinoyama, Isao; Kamikubo, Takashi; Toyoshima, Akira; Samizu, Kiyohiro; Kawaminami, Eiji; Imamura, Masakazu; Moritomo, Hiroyuki; Matsuhisa, Akira; Hirano, Masaaki; Miyazaki, Yoji; Nozawa, Eisuke; Okada, Minoru; Koutoku, Hiroshi; Ohta, Mitsuaki
PATENT ASSIGNEE(S): Yamanouchi Pharmaceutical Co., Ltd., Japan; et al.
SOURCE: PCT Int. Appl., 65 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000017163	A1	20000330	WO 1999-JP5149	19990921
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
CA 2345146	AA	20000330	CA 1999-2345146	19990921
AU 9956544	A1	20000410	AU 1999-56544	19990921
AU 754529	B2	20021121		
BR 9914018	A	20010703	BR 1999-14018	19990921
EP 1122242	A1	20010808	EP 1999-943446	19990921
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 3390744	B2	20030331	JP 2000-574073	19990921
JP 2003137873	A2	20030514	JP 2002-328498	19990921
CN 1129581	B	20031203	CN 1999-811198	19990921
RU 2221785	C2	20040120	RU 2001-107612	19990921
US 6673799	B1	20040106	US 2001-787672	20010321
US 2004010037	A1	20040115	US 2003-608341	20030630

PRIORITY APPLN. INFO.:	JP 1998-267508	A	19980922
	JP 1999-155398	A	19990602
	JP 2000-574073	A3	19990921
	WO 1999-JP5149	W	19990921
	US 2001-787672	A3	20010321

OTHER SOURCE(S): MARPAT 132:237107

GI



I

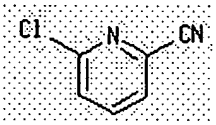
AB The title compds. I [T1 = (CH2)n; T2 = (CH2)k; T3 = (NR4Y)mR5; R = cyano, etc.; R1 = H, halo, etc.; R2 - R4 = H, alkyl, etc.; R5 = alkyl, etc.; k, n = 1 - 3; m = 0 or 1; X = CO, etc.; Z1, Z2 = CH, N; a proviso is given; Y = alkylene, etc.] are prepd. These derivs. exhibit antiandrogen activities and are therefore useful in the prevention or treatment of prostatic cancer, prostatic hypertrophy and so forth. In an in vitro assay for inhibition of androgen binding to androgen receptors, (2R,5S)-N-(2-bromo-4-pyridyl)-4-(4-cyano-3-trifluoromethylphenyl)-2,5-dimethylpiperazine-1-carboxamide showed the Ki value of 7.5 nM.

IT **33252-29-8**

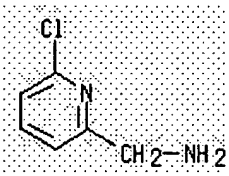
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of piperazino-substituted cyanophenyl derivs. as antiandrogen agents)

RN 33252-29-8 HCAPLUS

CN 2-Pyridinecarbonitrile, 6-chloro- (9CI) (CA INDEX NAME)



IT **188637-75-4P**, 2-Aminomethyl-6-chloropyridine
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of piperazino-substituted cyanophenyl derivs. as antiandrogen agents)
RN 188637-75-4 HCAPLUS
CN 2-Pyridinemethanamine, 6-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

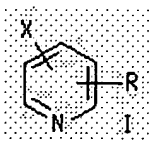
L11 ANSWER 28 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

Full Text | Citing References

ACCESSION NUMBER: 1998:236766 HCAPLUS
DOCUMENT NUMBER: 128:282788
TITLE: Preparation of (aminomethyl)pyridines from cyanopyridines
INVENTOR(S): Ueno, Toshiya; Kimura, Yoshikazu; Honta, Tomohiro; Kitasawa, Sadaya; Kimura, Osamu; Takuma, Yuki
PATENT ASSIGNEE(S): Nippon Fine Chemical Co., Ltd, Japan; Mitsubishi Chemical Industries Ltd.
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

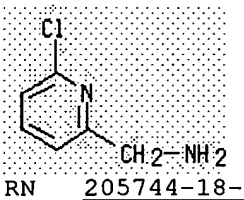
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10101646	A2	19980421	JP 1996-261865	19961002

PRIORITY APPLN. INFO.: JP 1996-261865 19961002
OTHER SOURCE(S): CASREACT 128:282788; MARPAT 128:282788
GI

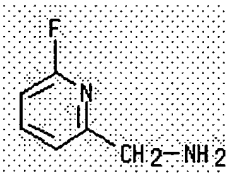


AB (Aminomethyl)pyridines I (R = CH2NH2; X = H, halo) are prepd. by hydrogenation of cyanopyridines I (R = cyano; X = same as above) in the presence of NH3 and Mn-contg. Raney catalysts. 2-Chloro-3-cyanopyridine was hydrogenated over Mn-contg. Raney Co in the presence of NH3/BuOH at 35? and 10 kg/cm^2 for 6 h to give 90.9% 2-chloro-3-aminomethylpyridine.
IT **188637-75-4P** **205744-18-9P**

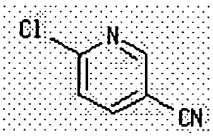
RL: IMF (Industrial manufacture); **PREP (Preparation)**
(prepn. of (aminomethyl)pyridines from cyanopyridines)
RN 188637-75-4 HCAPLUS
CN 2-Pyridinemethanamine, 6-chloro- (9CI) (CA INDEX NAME)



RN 205744-18-9 HCAPLUS
CN 2-Pyridinemethanamine, 6-fluoro- (9CI) (CA INDEX NAME)



IT **33252-28-7**, 2-Chloro-5-cyanopyridine
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(prepn. of (aminomethyl)pyridines from cyanopyridines)
RN 33252-28-7 HCAPLUS
CN 3-Pyridinecarbonitrile, 6-chloro- (9CI) (CA INDEX NAME)



L11 ANSWER 29 OF 29 HCAPLUS COPYRIGHT 2006 ACS on STN

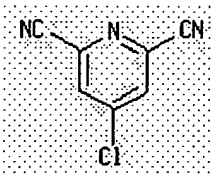
Full Text | Citing References

ACCESSION NUMBER: 1975:156097 HCAPLUS
DOCUMENT NUMBER: 82:156097
TITLE: 2,6-Bis(aminomethyl)pyridine
INVENTOR(S): Matsumoto, Ikuo; Kubo, Katsuo
PATENT ASSIGNEE(S): Inoue, Michiro; Shimamoto, Takio; Ishikawa, Masayuki; Ishikawa, Hisako
SOURCE: Jpn. Tokkyo Koho, 3 pp.
CODEN: JAXXAD
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

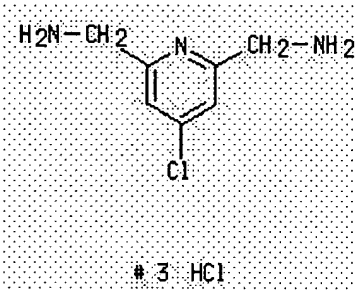
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 49040473	B4	19741102	JP 1970-86438	19701003

PRIORITY APPLN. INFO.: JP 1970-86438 19701003
GI For diagram(s), see printed CA Issue.
AB 2,6-Bis(aminomethyl)pyridine trihydrochlorides (I, R = H, Cl) were prepd. by hydrogenating the corresponding 2,6-dicyanopyridine in HCl-MeOH over Pd-C. E.g., a suspension of 5.16 g 2.6-dicyanopyridine in 100 ml MeOH was treated with 20 ml 40% HCl-MeOH and 1.5 g 10] Pd-C and 3 kg/cm^3 H at room temp. for ~10 min to give 9.3 g I (R = H).
IT **55306-66-6**

RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(catalytic hydrogenation of)
RN 55306-66-6 HCAPLUS
CN 2,6-Pyridinedicarbonitrile, 4-chloro- (9CI) (CA INDEX NAME)



IT **55306-67-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 55306-67-7 HCAPLUS
CN 2,6-Pyridinedimethanamine, 4-chloro-, trihydrochloride (9CI) (CA INDEX NAME)



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FILE 'REGISTRY' ENTERED AT 14:51:12 ON 15 MAY 2006
L1 STRUCTURE UPLOADED
L2 0 S L1
L3 64 S L1 FULL

FILE 'HCAPLUS' ENTERED AT 14:52:55 ON 15 MAY 2006
L4 56 S L3/PREP

FILE 'REGISTRY' ENTERED AT 14:53:02 ON 15 MAY 2006
L5 STRUCTURE UPLOADED
L6 19 S L5
L7 1726 S L5 FULL

FILE 'HCAPLUS' ENTERED AT 14:54:12 ON 15 MAY 2006
L8 983 S L7/RCT

FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 15 MAY 2006

FILE 'REGISTRY' ENTERED AT 14:54:31 ON 15 MAY 2006

FILE 'HCAPLUS' ENTERED AT 14:54:37 ON 15 MAY 2006
L9 30 S L8 AND L4
L10 1 S L9 AND VANGELISTI, M?/AU
L11 29 S L9 NOT L10

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=> s l3 and l7
            82 L3
          1311 L7
L12           33 L3 AND L7

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                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   176.07     519.51

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -22.50     -22.50

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FILE COVERS 1907-1966
FILE LAST UPDATED:  01 May 1997 (19970501/UP)

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  assignees, and patent information, e.g., patent numbers, are
  now searchable from 1907-1966.  TIFF images of CA abstracts
  printed between 1907-1966 are available in the PAGE
  display formats.

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  all substance data from the REGISTRY file.  Enter HELP FIRST for
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L1              STRUCTURE UPLOADED
L2            0 S L1
L3           64 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:52:55 ON 15 MAY 2006
L4           56 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:53:02 ON 15 MAY 2006
L5              STRUCTURE UPLOADED
L6           19 S L5
L7         1726 S L5 FULL

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L8          983 S L7/RCT

     FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 15 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:54:31 ON 15 MAY 2006

     FILE 'HCAPLUS' ENTERED AT 14:54:37 ON 15 MAY 2006
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L9            30 S L8 AND L4
L10            1 S L9 AND VANGELISTI, M?/AU
L11           29 S L9 NOT L10
L12           33 S L3 AND L7

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              0 L3
             41 L7
L13           0 L3 AND L7

=>
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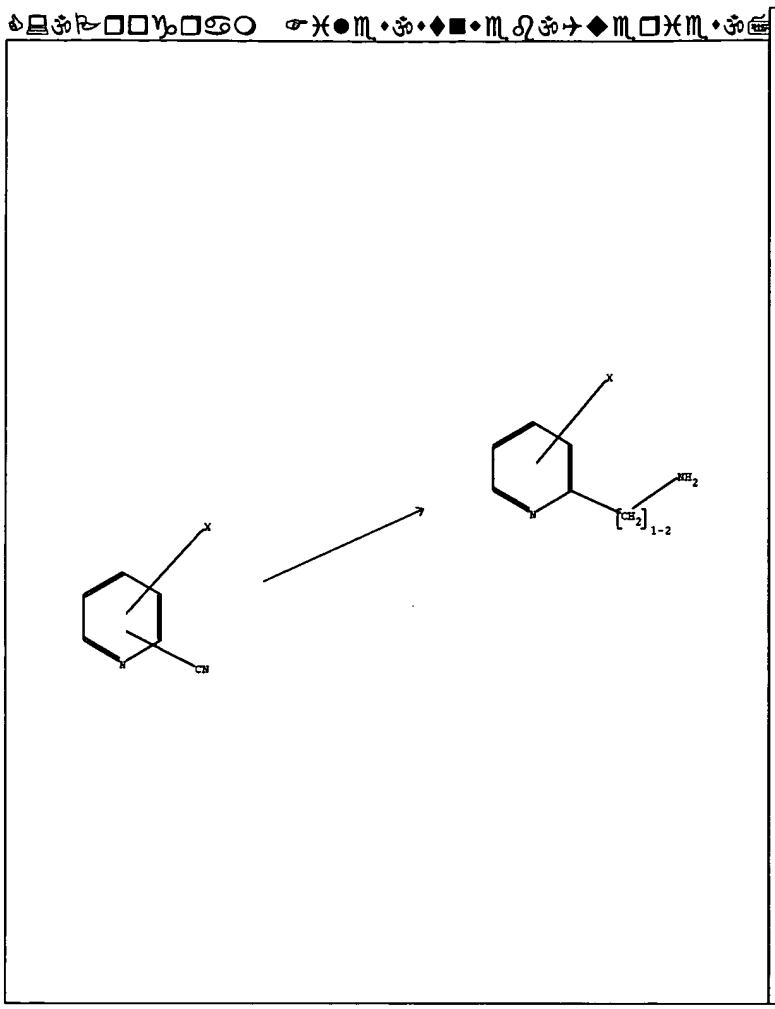
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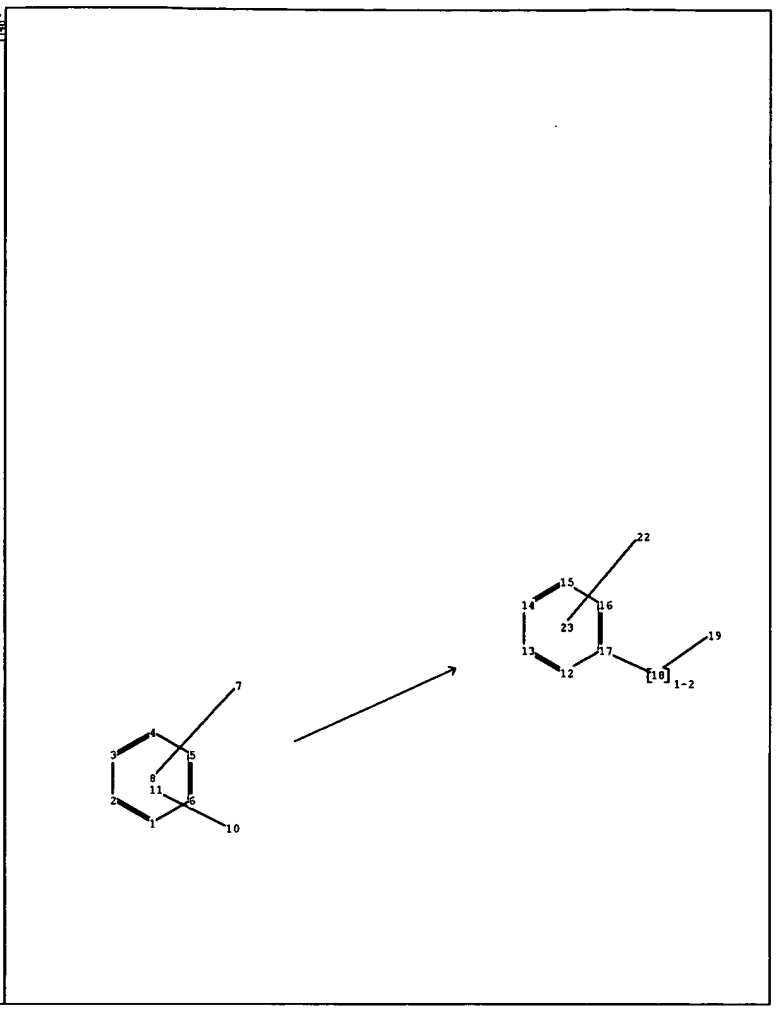
CN
X
NH2
[CH2]1-2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4
3
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11
2
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1
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14
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23
13
12
17
19
[10]1-2

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=> d his

     (FILE 'HOME' ENTERED AT 14:51:04 ON 15 MAY 2006)

     FILE 'REGISTRY' ENTERED AT 14:51:12 ON 15 MAY 2006
L1             STRUCTURE UPLOADED
L2               0 S L1
L3              64 S L1 FULL

     FILE 'HCAPLUS' ENTERED AT 14:52:55 ON 15 MAY 2006
L4              56 S L3/PREP

     FILE 'REGISTRY' ENTERED AT 14:53:02 ON 15 MAY 2006
L5             STRUCTURE UPLOADED
L6              19 S L5
L7            1726 S L5 FULL

     FILE 'HCAPLUS' ENTERED AT 14:54:12 ON 15 MAY 2006
L8             983 S L7/RCT

     FILE 'HCAPLUS' ENTERED AT 14:54:19 ON 15 MAY 2006

     FILE 'REGISTRY' ENTERED AT 14:54:31 ON 15 MAY 2006

     FILE 'HCAPLUS' ENTERED AT 14:54:37 ON 15 MAY 2006
L9              30 S L8 AND L4
L10              1 S L9 AND VANGELISTI, M?/AU
L11             29 S L9 NOT L10
L12             33 S L3 AND L7

     FILE 'CAOLD' ENTERED AT 15:00:03 ON 15 MAY 2006
L13              0 S L3 AND L7

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L14            STRUCTURE UPLOADED
L15              0 S L14
L16              4 S L14 FULL

=> d l16, abs fhit rx, 1-4


L16  ANSWER 1 OF 4  CASREACT  COPYRIGHT 2006 ACS on STN
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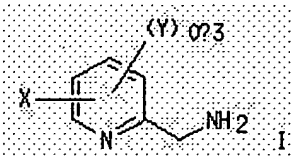
Citing References

GI

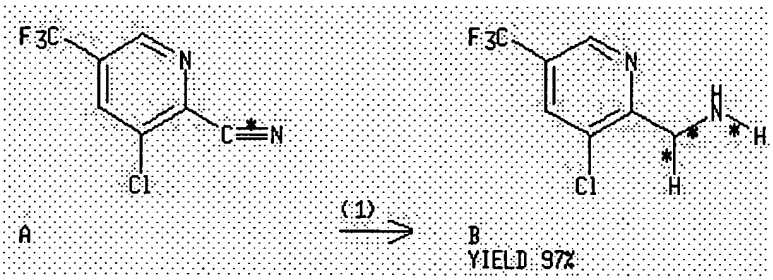


I

AB The invention relates to a process for the prepn. of 2-aminomethylpyridine derivs. of formula I [wherein: X is halogen atom; each Y may be the same or different and may be a halogen atom, a halogenoalkyl, an alkoxycarbonyl or an alkylsulfonyl], useful as intermediates for prepn. of pesticides. 2-Aminomethyl-3-chloro-5-trifluoromethylpyridine was prepd. via Raney Ni-catalized hydrogenation of 2-cyano-3-chloro-5-trifluoromethylpyridine with a yield of 97%. The advantages of the proposed prepn. of

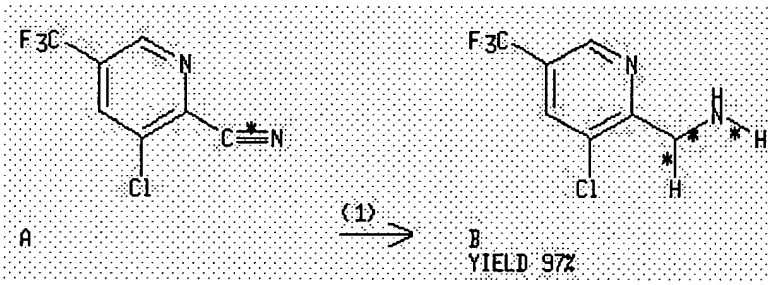
2-aminomethylpyridine derivs. include the use of Raney nickel catalyst instead of expensive Pd catalyst (the Pd-catalized hydrogenation suffers from the disadvantage of dehalogenation reaction; Pd is also very sensitive to catalysts poisons).

RX(1) OF 1 **A** ===> **B**



RX(1) RCT A **80194-70-3**
RGT C 1333-74-0 H2
PRO B **175277-74-4**
CAT 7440-02-0 Ni
SOL 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C, pH 7
SUBSTAGE(2) 2 hours, 40 deg C, 18 bar, pH 7
NTE Raney nickel used

RX(1) OF 1 **A** ===> **B**



RX(1) RCT A **80194-70-3**
RGT C 1333-74-0 H2
PRO B **175277-74-4**
CAT 7440-02-0 Ni
SOL 64-19-7 AcOH
CON SUBSTAGE(1) room temperature -> 40 deg C, pH 7
SUBSTAGE(2) 2 hours, 40 deg C, 18 bar, pH 7
NTE Raney nickel used

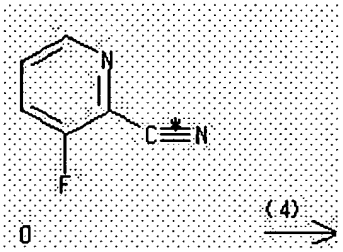
L16 ANSWER 2 OF 4 CASREACT COPYRIGHT 2006 ACS on STN

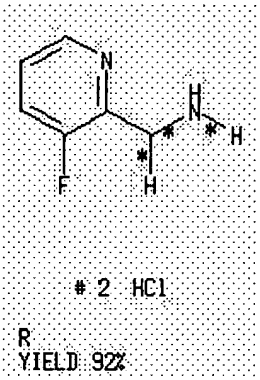
Clinical References

AB A scaleable route to 2-{3-[(2,2-difluoro-2-(2-pyridyl)ethyl)amino]-6-chloro-2-oxohydropyrazinyl}-N-[(3-fluoro(2-pyridyl))methyl]acetamide (I) is described in which various scaleup issues were addressed to provide a safe, efficient, and robust route for the prepn. of multi-kilo amts. of

the compd. The use of expensive and toxic reagents, notably sodium azide, TMS-cyanide, and Deoxo-Fluor, and the need for specialist equipment were overcome in the prepn. of the key fluorinated intermediates 2,2-difluoro-2-(2-pyridyl)ethylamine and 2-aminomethyl-3-fluoropyridine. With minimal isolations and through processing of intermediates, the thrombin inhibitor I was isolated in 36% overall yield.

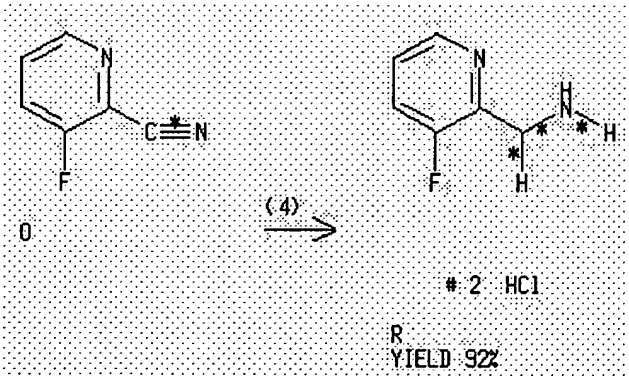
RX(4) OF 84 ...O ===> R...





RX(4) RCT O **97509-75-6**
RGT S 7647-01-0 HCl, T 1333-74-0 H2
PRO R **312904-49-7**
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 18 hours, 20 deg C, 5 psi

RX(4) OF 84 ...O ===> R...



RX(4) RCT O **97509-75-6**
RGT S 7647-01-0 HCl, T 1333-74-0 H2
PRO R **312904-49-7**

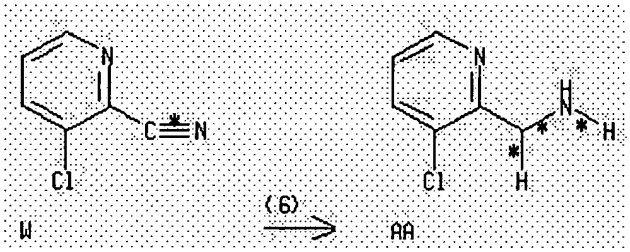
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH
CON 18 hours, 20 deg C, 5 psi

L16 ANSWER 3 OF 4 CASREACT COPYRIGHT 2006 ACS on STN

Citing References

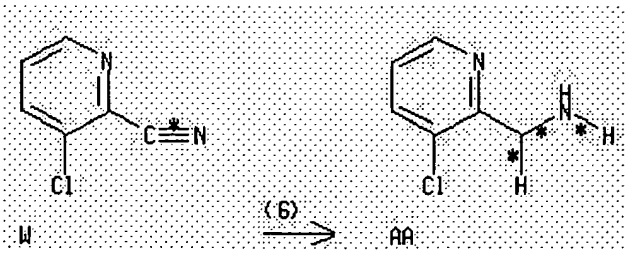
AB Recent efforts in the field of thrombin inhibitor research have focused on the identification of compds. with good oral bioavailability and pharmacokinetics. In this manuscript we describe a metab.-based approach to the optimization of the 3-(2-phenethylamino)-6-methylpyrazinone acetamide template which resulted in the modification of each of the three principal components (i.e., P1, P2, P3) comprising this series. As a result of these studies, several potent thrombin inhibitors were identified which exhibit high levels of oral bioavailability and long plasma half-lives.

RX(6) OF 261 ...**W** ===> **AA**...



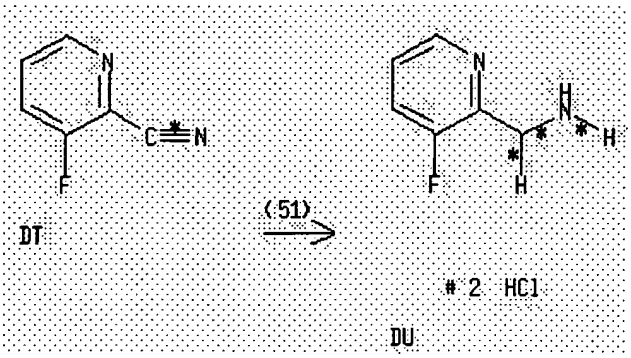
RX(6) RCT W **38180-46-0**
RGT AB 1333-74-0 H2, AC 7664-41-7 NH3
PRO AA **500305-98-6**
CAT 7440-02-0 Ni
SOL 64-17-5 EtOH
CON 5 hours, 1 atm
NTE Raney nickel used

RX(6) OF 261 ...**W** ===> **AA**...



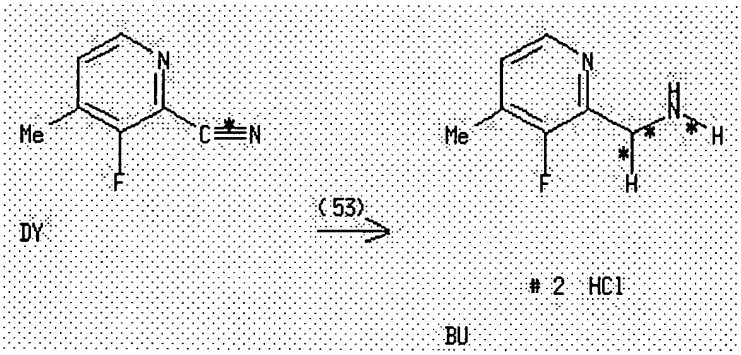
RX(6) RCT W **38180-46-0**
RGT AB 1333-74-0 H2, AC 7664-41-7 NH3
PRO AA **500305-98-6**
CAT 7440-02-0 Ni
SOL 64-17-5 EtOH
CON 5 hours, 1 atm
NTE Raney nickel used

RX(51) OF 261 **DT** ===> **DU**



RX(51) RCT DT **97509-75-6**
RGT I 7647-01-0 HCl, AB 1333-74-0 H2
PRO DU **312904-49-7**
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH, 7732-18-5 Water
CON 16 hours, 40 psi

RX(53) OF 261 **DY** ===> **BU**...



RX(53) RCT DY **312904-99-7**
RGT I 7647-01-0 HCl, AB 1333-74-0 H2
PRO BU **312905-00-3**
CAT 7440-05-3 Pd
SOL 64-17-5 EtOH, 7732-18-5 Water
CON 16 hours, 55 psi

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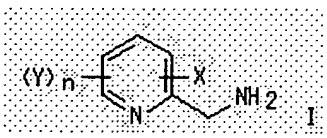
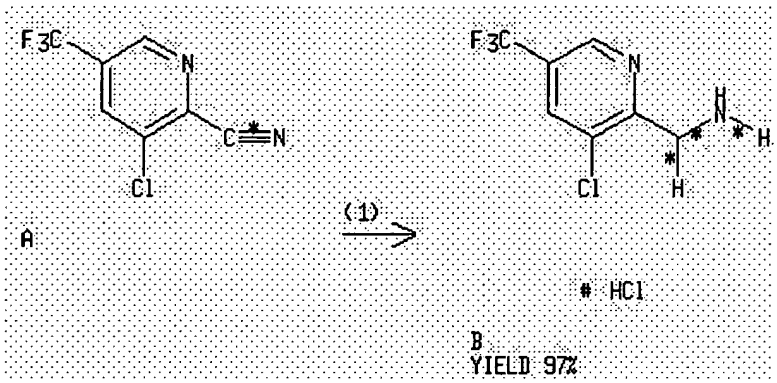
Citing References

GI



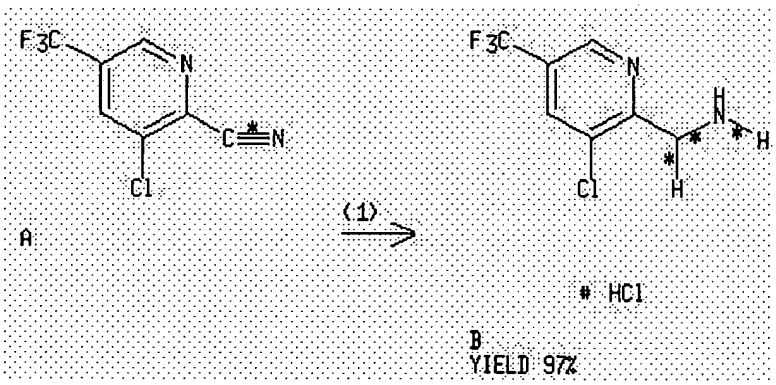
AB Title compds. (I; X = halo; Y = halo, haloalkyl, alkoxycarbonyl, alkylsulfonyl; n = 0-3) were prepd. by catalytic hydrogenation of the corresponding 2-cyano derivs. Thus, 3-chloro-2-cyano-5-trifluoromethylpyridine (prepn. given) was hydrogenated in MeOH over Pd/C contg. HCl at 1 atm. to give 95-97% 2-aminomethyl-3-chloro-5-trifluoromethylpyridine hydrochloride.

RX(1) OF 1 **A** ===> **B**



RX(1) RCT A **80194-70-3**
RGT C 1333-74-0 H2, D 7647-01-0 HCl
PRO B **326476-49-7**
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

RX(1) OF 1 **A** ===> **B**



RX(1) RCT A **80194-70-3**
RGT C 1333-74-0 H2, D 7647-01-0 HCl
PRO B **326476-49-7**
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH

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